

Electronic Supplementary Information

**Influence of Linkers on the Kuratowski-type Secondary Building Unit
in Nickel Single-site MOFs for Ethylene Oligomerization Catalysis: A
Computational Study**

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Periodic Calculations

Geometry optimizations of the periodic unit cells of Ni-MFU-4l and Ni-CFA-1 MOFs were performed using DFT periodic boundary conditions as implemented in VASP simulation package.¹ Periodic DFT calculations were optimized at the PBE-D3² level and the projector-augmented wave (PAW)³ pseudopotentials employing 500 eV kinetic energy cutoff and 1x1x1 k-points.

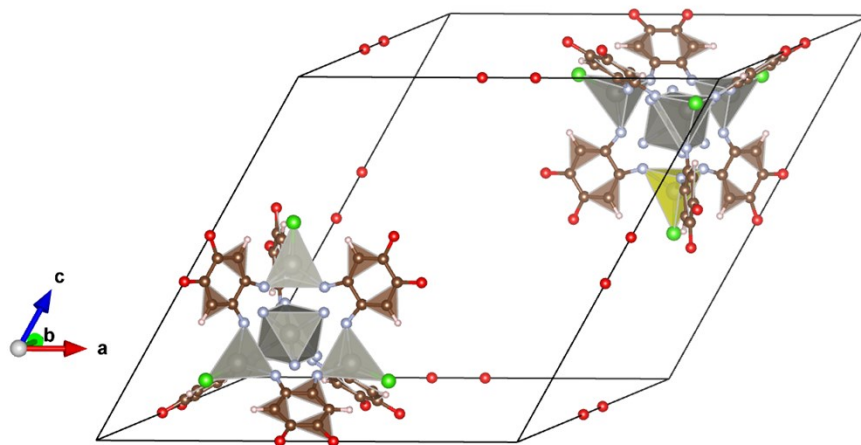


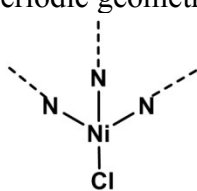
Figure S1. Periodic structure of Ni-MFU-4l optimized at the PBE-D3 level of theory.

Method Validation

A preliminary study of different DFT functionals has been carried out in order to compare the periodic geometry of the secondary building unit of Ni-MFU-4l MOF (see Table S1). The validation of the functional is extremely important since each of them depends on the application and may be different for the study of energies (bond, interaction, transition state, relative energies, etc.) and molecular structures. Among DFT functionals that have proven to be useful in the study of MOFs, the M06-L functional stand out,⁴ which has a good performance in the reproduction of experimental trends.⁵ Furthermore, it has recently been used with good results in thermochemical and kinetic studies of the ethylene dimerization process supported on the secondary building unit of NU-1000.^{6, 7} However, this functional accounts for the dispersion effects in a semi-quantitative way for medium-

range correlation energy, so it cannot predict dispersion in long-range regions without overlap. This explains why the functional M06-L deviates from the periodic geometric parameters of Ni-MFU-4l (see Table S1). Long-range dispersion corrections have been reported in MOFs to be essential to stabilize structures and, in some cases, to converge the system to a geometry that is consistent with the periodic structure.⁵ The hybrid functionals B3LYP-D3⁸⁻¹⁰ and M06-2X¹¹ are other examples used in the study of MOFs, the former being one of the most popular hybrid methods in the study of gas adsorption and storage in MOFs.⁵ Despite this, the functionals based on generalized gradients (GGA) seem to be the most appropriate for our case (see Table S1). PBE0¹² and BP86^{5, 8-10, 13} are functionals that attempt to separately approximate electronic interchange and correlation while being less computationally expensive, which is highly advantageous. The PBE0 functional uses 25% exact exchange and 75% DFT exchange, which combined with D3BJ-correction (as shown in Table S1) works quite well to predict the secondary building unit structure of Ni-MFU-4l compared to the periodic parameters. This result is further supported by a recent study on the successful characterization of various metal-organic structures with GGA methods.¹⁴

Table S1. Comparison of geometric parameters of the catalytically active center of Ni-MFU-4l with different DFT functionals. All calculations were performed in the Gaussian program16 using def2-SVP basis set for the atoms of H, C, O, N, and Cl, and def2-TZVP for Zn, while the SDD pseudopotential was used to describe the Ni reactive center.

Method	d-Ni-N	d-Ni-Cl	∠N-Ni-N	∠N-Ni-Cl
Periodic geometry 	1.945 Å	2.121 Å	97.06°	120.07°
PBE0-D3BJ	1.967 Å	2.150 Å	96.54°	120.53°
BP86-D3BJ	1.985 Å	2.164 Å	96.65°	120.40°
M06-L	2.019 Å	2.182 Å	95.01°	121.64°
B3LYP-D3	2.019 Å	2.183 Å	96.45°	120.55°
M06-2X	2.030 Å	2.161 Å	98.56°	118.93°

CFA-1 MOF coordination environments

CFA-1 is constructed from $\text{Zn}_5\text{Cl}_4(\text{H}_2\text{-bibta})_6$ secondary building units interconnected by achiral linkers. Therefore, this MOF structure breaks the Kuratowski-type secondary building unit's symmetry, and thus not all of the pore-exposed have identical tetrahedral Zn sites. The four peripheral Zn (II) ions show two different local coordination environments, as shown in Figure S2. Coordination site 1, is repeated for three of the peripheral Zn (II) ions of the secondary building unit of this MOF, while site 2 is present in a single site of the secondary building unit. Experimentally, the complete exchange of all four peripheral Zn (II) ions requires an excess of Ni (II) ions in solution because depending on the Ni/Zn molar ratio, different numbers of Zn sites could be replaced. In contrast, the octahedrally coordinated Zn site cannot be replaced. The Dinca group used a low loading of Ni (<7.5%) to exchange only one site of the four peripheral Zn environments behaving as a single-site platform catalytically active for ethylene coordination.¹⁵ However, there is no experimental evidence on the exact location of the exchanged metal ions on this MOF, and thus which site is most favored for a metal ion exchange. According to Li and co-workers, some important aspects to consider are; the first coordination sphere in which the metal ion is weakly bound to a ligand, the reaction conditions, and the diffusibility of the metal ions entering the MOF.¹⁶ From this perspective, it could be assumed that site 1, sterically open, could be more favored for the diffusion of metal ion exchange. This is only an assumption since the mechanism of metal ion exchange reaction is not fully studied and understood.

We have computed the binding energies in these two different environment coordination sites of CFA-1 as shown in Figure S2, exchanging one of the Zn ions for Ni and the chloride for ethyl, considering two types of active species. The computed binding energies were -11.8 and -9.3 kcal/mol for sites 1 and 2, respectively. This result is not a surprise since the coordination environment site 1 is more sterically open than site 2. Additionally, we performed an EDA analysis of the π -complex geometries (II) of both sites (Table S2) in order to compare their reactivity with the substrate. Surprisingly, we have found the same values of interaction energy (ΔE_{int}) in the π -complex for both coordination environments with a similar trend of the non-covalent interactions (see Table S2). One of the main

differences between both sites is the Pauli energy term (ΔE_{Pauli}), which is slightly higher (in 1.9 kcal/mol) for site 2 in line with their less favorable binding energy. While dispersion (ΔE_{disp}) and electrostatic (ΔE_{elstat}) interactions in site 1 slightly decreased due to a lower interaction of the linker with the monomer due to their less sterically site than site 2. Therefore, site 2 is stabilized by slightly dispersive and electrostatic attraction with the substrate, compensating their greater steric effect, which further suggests that through the compensation of these effects on site 2, both sites' reactivity with the substrate are practically the same.

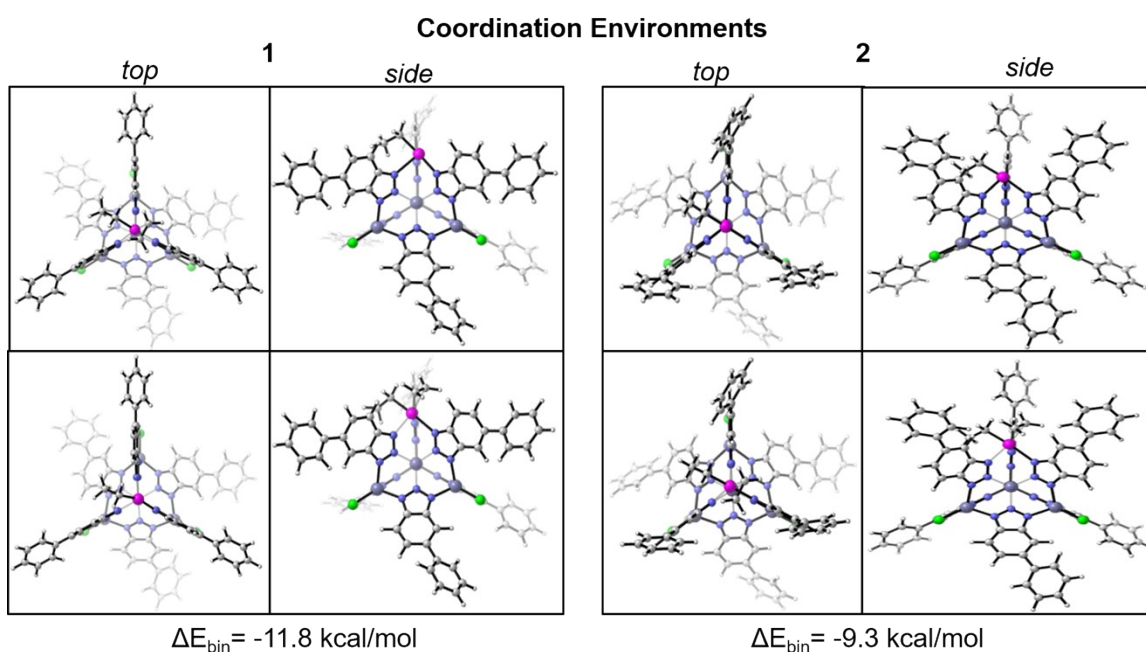


Figure S2. The top and side views of CFA-1 MOF coordination environment cluster models.

Table S2. Energy decomposition analysis, according to Eq. 1 (main manuscript), for the π -complex geometry I1. ΔE energy term is the energy difference between the Ni-catalyst and the ethylene molecule according to Figure S2. All values are in kcal/mol.

<i>Energy term</i>	<i>1</i>	<i>2</i>
ΔE_{int}	-54.6	-54.6
ΔE_{Pauli}	164.6 (43%)	166.5 (43%)
ΔE_{disp}	-40.0 (10%)	-40.8 (11%)
ΔE_{elstat}	-138.4 (36%)	-139.8 (36%)
ΔE_{pol}	-32.4 (9%)	-32.5 (8%)
ΔE_{ct}	-8.4 (2%)	-8.0 (2%)

Finally, we also study the free energy barriers of the determining-transition states (TS-I1) for both coordination environments (Table S3). The calculations revealed that the more sterically demanding site 2 binds to the ethylene by less favorable coordination ($\Delta G^\circ=2.1$ kcal/mol), whereas the free energy barrier (ΔG^\ddagger) of site 2 is slightly more stable than site 1 by 1.2 kcal/mol. These results suggest that site 1 is more favorable than site 2 in the thermodynamic aspect, while site 2 is more favorable in the kinetic one. This latter is probably due to site 2 geometry has a closer distance between the linker and the substrate, and their non-covalent dispersive and electrostatic interactions may play a more significant role in the activity, which is similar to the trend of the coordination environment of the high-performance homogeneous industrial catalyst (TpMes)NiCl¹⁷ (site 2; Figure S2), and thus, it is interesting to explore this most similar environment on the ethylene oligomerization catalysis.

Table S3. Gibbs free energies of the π -complexes (I1) and determining-transition states (TS-I1) for the coordination environments 1 and 2 of CFA-1 cluster model according to Figure S2.

<i>Coordination environment</i>	<i>1</i>	<i>2</i>
ΔG° (I1)	2.4	4.5
ΔG^\ddagger (TS-I1)	28.2	27.0

DFT cluster model of the Kuratowski-type secondary building unit

The mechanistic studies have been carried out using a cluster model, the Kuratowski-type secondary building unit extracted from each MOF structure's periodic unit cell. The active species AE1 were modeled from their periodic geometries, replacing one Zn and Cl atom from the tetrahedral environment with one Ni atom and ethyl molecule. The positions of all atoms were optimized at PBE0-D3BJ level except for the bis-triazolate linkers to mimic each structure's framework rigidity.

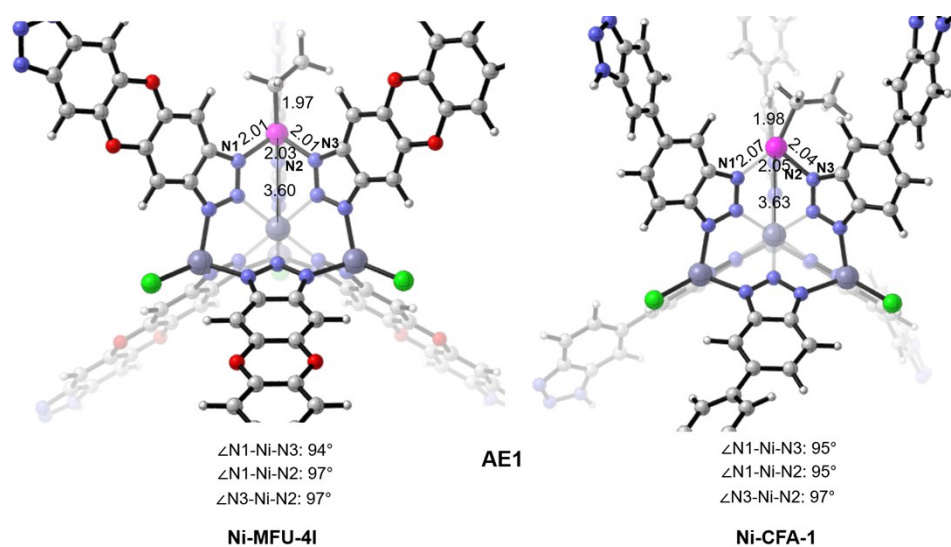


Figure S3. Computed AE1 active species for Ni-MFU-4l and Ni-CFA-1 complexes. Color code: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen), green (chlorine), petrol blue (zirconium) and pink (nickel). Distances are in angstrom (Å).

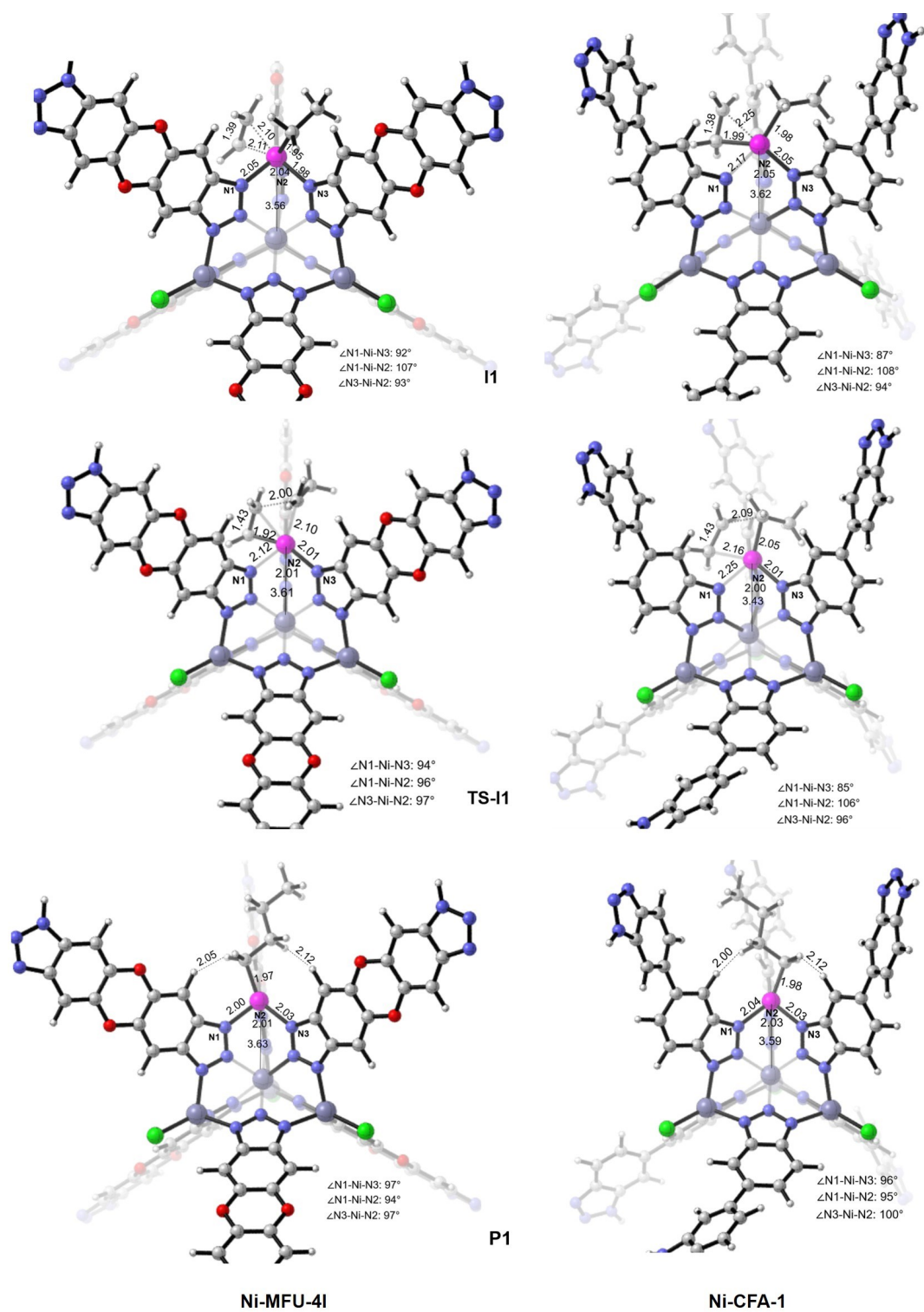


Figure S4. Optimized structures and bond distances (Å) of intermediates and transition states associated with the first ethylene insertion step.

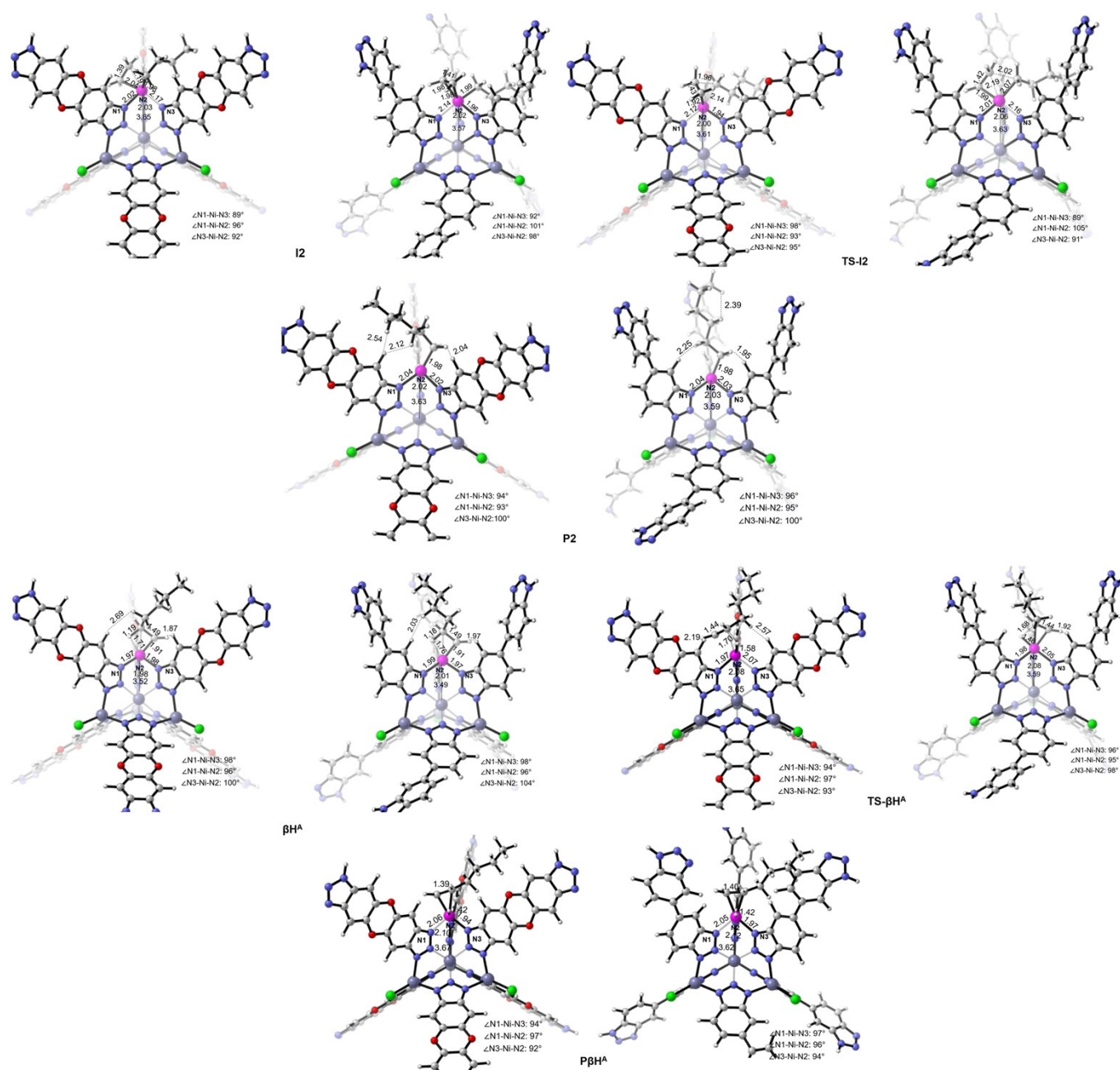


Figure S5. Optimized structures and bond distances (Å) of intermediates and transition states associated with the reaction path A.

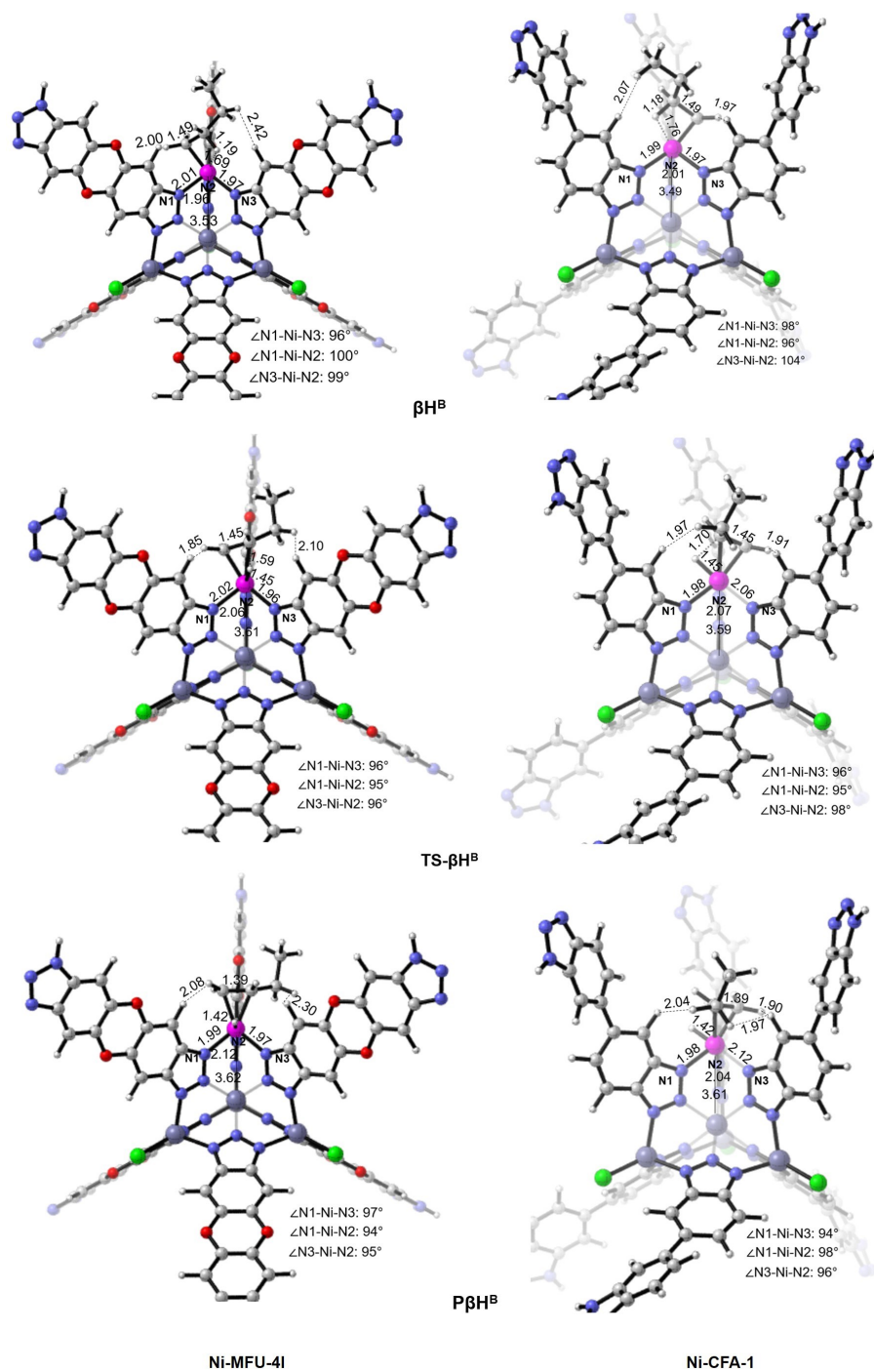


Figure S6. Optimized structures and bond distances (Å) of intermediates and transition states associated with the reaction path B.

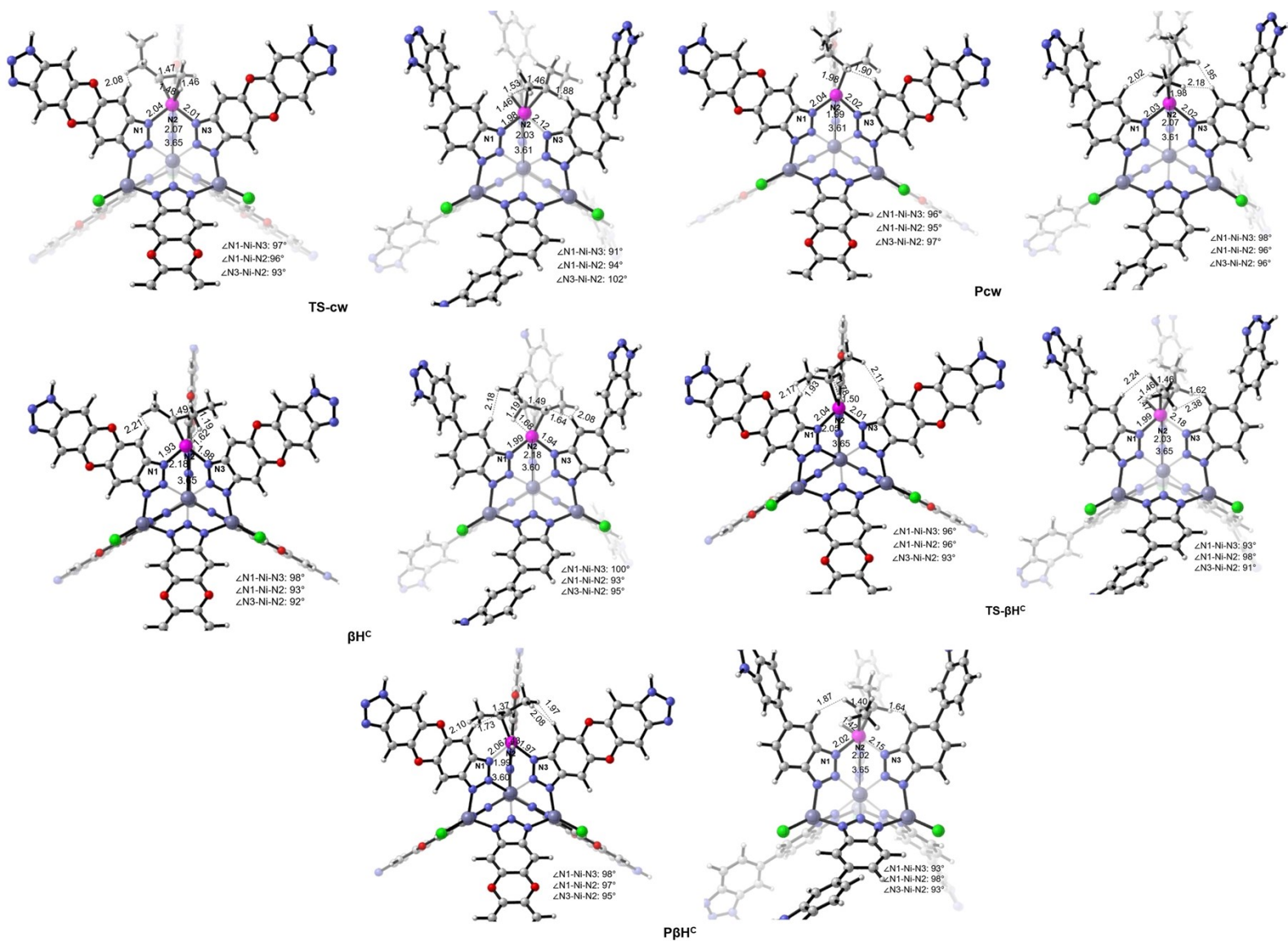


Figure S7. Optimized structures and bond distances (Å) of intermediates and transition states associated with the reaction path C.

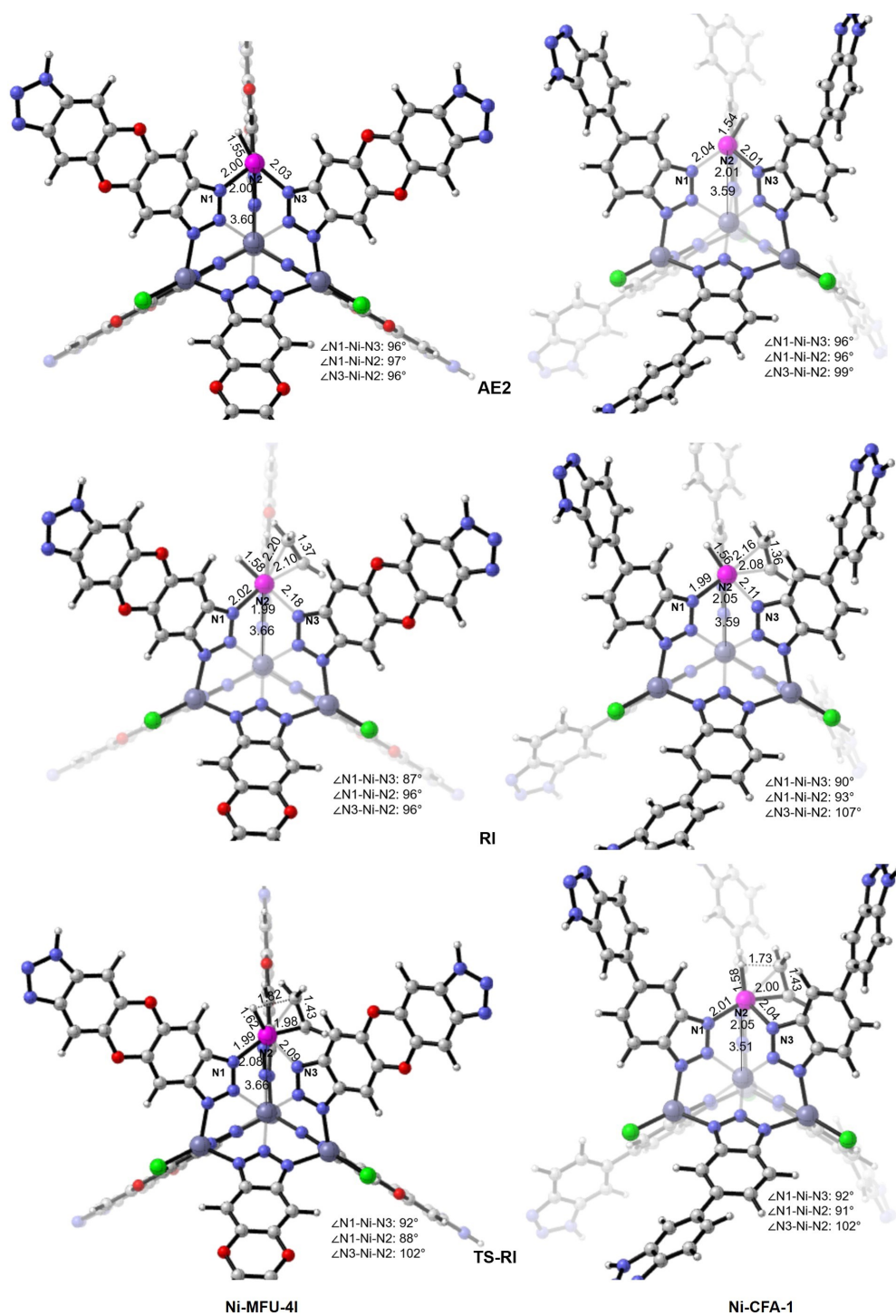


Figure S8. Optimized structures and bond distances (Å) of intermediates and transition states associated with the ethylene reinsertion on nickel-hydride complex.

Temperature effect

Experimentally Ni-MFU-4l catalyst at 50 °C (323 K) the catalytic activity is much lower ($1,700\text{ h}^{-1}$) than at room temperature ($41,500\text{ h}^{-1}$) under the same conditions (50 bar in toluene and presence of MAO), while the selectivity at 1-butene decreases from 92% to 70%, with an increase in the selectivity towards 1-hexene of 13% concerning the 3% obtained at 25 °C (298 K).¹⁸ A similar trend is observed for Ni-CFA-1.¹⁵ Therefore, increasing the temperature increases the probability of getting higher chain growth, although 1-butene is still the main product. Based on this experimental evidence, we evaluate the effect of temperature on activity and selectivity. We have only considered evaluating the free energies associated with the Ni-MFU-4l catalyst for comparative purposes, as shown in Figure S8. Our calculations confirm the observed temperature dependence of the activity where the rate-determining step reaches a free energy barrier of 26 kcal/mol, which is 1.2 kcal/mol higher than the computed barrier at room temperature. On the other hand, although the step from P1 to I2 continues to be thermodynamically unfavorable, the effect of temperature is notorious since it is less endergonic when it reaches 50 °C (+6.6 kcal/mol) concerning 25 °C (+7.6 kcal/mol), and thus being chain propagation is more likely at 50 °C in agrees with the experimental evidence. While the computed step from P1 to βH^{B} are practically similar (3.3 vs. 3.4 kcal/mol at 50°C and 25°C, respectively) although the stability of the intermediate βH^{B} is lower with increasing temperature (see Figure S8). In terms of selectivity, the energy difference between the activation free energy ($\Delta\Delta G^\ddagger$) of the determining transition states associated with each reaction path (TS-I2 and TS- βH^{B}) showed that the selectivity towards 1-butene prevails over the chain oligomerization at a higher temperature. However, the computed selectivity also indicates an elevated temperature can induce a slight increase in the chain growth in agreement with the experiment.

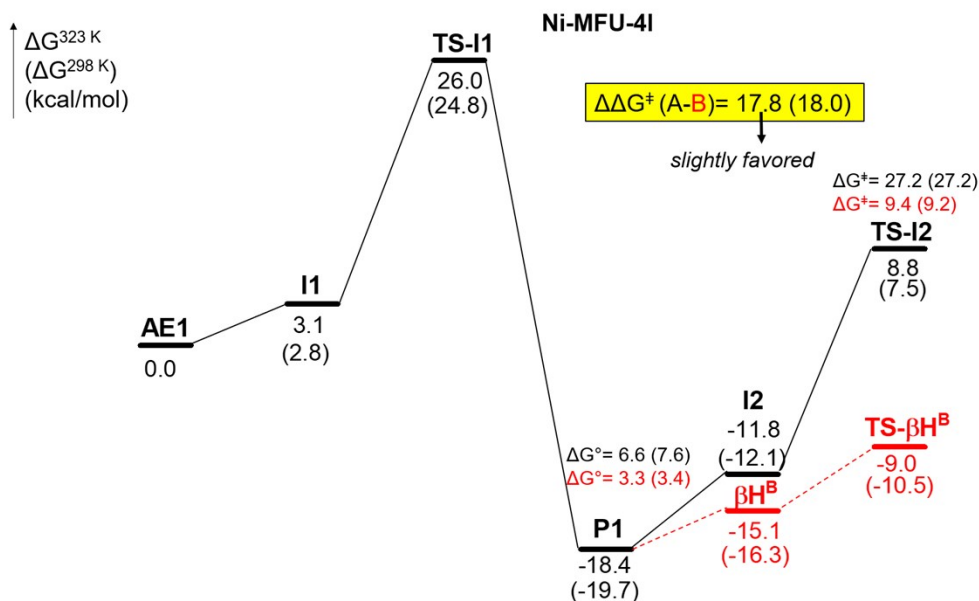


Figure S9. Computed Gibbs free energy profiles for the 1-hexene; pathway A (black), 1-butene; pathway B (red) in toluene with Ni-MFU-4l catalyst. $\Delta\Delta G^\ddagger$ is the activation free energy difference between the free energy barriers (ΔG^\ddagger) associated with the determining transition states; TS-I2 and TS-βH^B.

Table S4. SCF (E), enthalpies (H), and Gibbs free energies (G) and imaginary frequencies of the optimized intermediates and transition state structures for Ni-MFU-4l complex in the gas phase.

T(298K)						
A/B/C	<S ² >	E (a.u.)	H (a.u.)	G (a.u.)	G _{corr} (a.u.)	<i>i</i> -frequency
AE1	0.0	-14371.86833	-	-	-	
	2.008	-14371.87185	-14371.76888	-14371.83911	-14371.83869	
I1	0.0	-14450.30504	-14450.14542	-14450.22674	-14450.22161	
	2.007	-14450.29611	-	-	-	
TS-I1	0.0	-14450.26678	-14450.11052	-14450.18701	-14450.18566	-467.3608
	2.008	-14450.24061	-	-	-	-450.4331
P1	0.0	-14450.32126	-	-	-	
	2.008	-14450.34129	-14450.18031	-14450.25793	-14450.25505	
I2	0.0	-14528.76237	-14528.53414	-14528.64333	-14528.64143	
	2.007	-14528.74022	-	-	-	
TS-I2	0.0	-14528.73425	-14528.49686	-14528.60507	-14528.60311	-452.5811
	2.008	-14528.70041	-	-	-	-423.0041
P2	0.0	-14528.77760	-	-	-	

	2.009	-14528.80723	-14528.58819	-14528.67101	-14528.66747	
βH^{A}	0.0	-14528.80273	-14528.58396	-14528.66424	-14528.66106	
	2.008	-14528.78967	-	-	-	
TS- βH^{A}	0.0	-14528.74546	-	-	-	-617.0123
	2.008	-14528.75638	-14528.54301	-14528.62525	-14528.62205	-516.7187
$\text{P}\beta\text{H}^{\text{A}}$	0.0	-14528.80093	-14528.58396	-14528.66499	-14528.66148	
	2.007	-14528.78472	-	-	-	
AE2	0.0	-14293.4626	-	-	-	
	2.008	-14293.47083	-14293.40976	-14293.45029	-14293.44929	
RI	0.0	-14371.87826	-14371.77689	-14371.84288	-14371.84288	
	2.009	-14371.86115	-	-	-	
TS-RI	0.0	-14371.84348	-	-	-	-681.002
	2.013	-14371.85306	-14371.75558	-14371.82082	-14371.82057	-626.523
βH^{B}	0.0	-14450.33753	-14450.17683	-14450.25110	-14450.24908	
	2.008	-14450.32281	-	-	-	
TS- βH^{B}	0.0	-14450.32705	-14450.16942	-14450.24227	-14450.24098	-608.3363
	2.008	-14450.30632	-	-	-	-563.022
$\text{P}\beta\text{H}^{\text{B}}$	0.0	-14450.33595	-14450.17655	-14450.24899	-14450.24813	
	2.009	-14450.31588	-	-	-	
TS-cw	0.0	-14450.32309	-14450.16552	-14450.23847	-14450.23748	-719.043
	2.007	-14450.28254	-	-	-	-691.002
Pcw	0.0	-14450.30881	-	-	-	
	2.008	-14450.32495	-14450.17432	-14450.25082	-14450.24935	
βH^{C}	0.0	-14450.34021	-14450.17953	-14450.25282	-14450.25242	
	2.009	-14450.32653	-	-	-	
TS- βH^{C}	0.0	-14450.31954	-14450.16215	-14450.23411	-14450.23353	-694.9607
	2.002	-14450.30496	-	-	-	-682.7213
$\text{P}\beta\text{H}^{\text{C}}$	0.0	-14450.33345	-14450.17280	-14450.24666	-14450.24519	
	2.008	-14450.32596	-	-	-	

Table S5. SCF (E), enthalpies (H), and Gibbs free energies (G) and imaginary frequencies of the optimized intermediates and transition state structures for Ni-CFA-1 complex.

T(298K)						
A/B/C	$\langle\text{S}^2\rangle$	E(a.u.)	H (a.u.)	G (a.u.)	G_{corr} (a.u.)	i -frequency
AE1	0.0	-13477.938342	-	-	-	
	2.008	-13477.95266	-13477.85986	-13477.9192	-13477.9185	
II	0.0	-13556.38326	-13556.25339	-13556.31565	-13556.31533	
	2.008	-13556.37022	-	-	-	
TS-II	0.0	-13556.33502	-13556.21617	-13556.27846	-13556.27785	-208.847

	2.007	-13556.323955	-	-	-	-258.095
P1	0.0	-13556.378744				
	2.008	-13556.41376	-13556.25306	-13556.32954	-13556.32730	
I2	0.0	-13634.84895	-13634.63082	-13634.71037	-13634.70789	
	2.009	-13634.83579	-	-	-	
TS-I2	0.0	-13634.81807	-13634.60068	-13634.67170	-13634.67070	-269.087
	2.008	-13634.796476	-	-	-	-323.112
P2	0.0	-13634.86338	-	-	-	
	2.003	-13634.877963	-13634.65898	-13634.74250	-13634.73823	
βH^{A}	0.0	-13634.884643	-13634.66601	-13634.74713	-13634.74349	
	2.008	-13634.863057	-	-	-	
TS- βH^{A}	0.0	-13634.870399	-13634.65511	-13634.73512	-13634.73186	-500.958
	2.009	-13634.855026				-606.328
P βH^{A}	0.0	-13634.874370	-13634.65734	-13634.73757	-13634.73437	
	2.008	-13634.860226	-	-	-	
AE2	0.0	-13399.452955	-	-	-	
	2.008	-13399.486585	-13399.46734	-13399.52711	-13399.52711	
RI	0.0	-13477.957700	-13477.85639	-13477.92220	-13477.92220	
	2.009	-13477.940363	-	-	-	
TS-RI	0.0	-13477.938609	-	-	-	-678.114
	2.008	-13477.941159	-13477.84388	-13477.90269	-13477.90242	-662.422
βH^{B}	0.0	-13556.418914	-13556.25836	-13556.33275	-13556.33072	
	2.009	-13556.382913	-	-	-	
TS- βH^{B}	0.0	-13556.407014	-13556.24957	-13556.32196	-13556.32088	-458.9427
	2.009	-13556.389624	-	-	-	-573.9211
P βH^{B}	0.0	-13556.411201	-13556.25192	-13556.32429	-13556.32327	
	2.009	13556.37858	-	-	-	
TS-cw	0.0	-13556.398394	-13556.24133	-13556.31375	-13556.31283	-719.8062
	2.008	-13556.379574	-	-	-	-687.561
Pcw	0.0	-13556.383021	-	-	-	
	2.008	-13556.418697	-13556.25827	-13556.33617	-13556.33310	
βH^{C}	0.0	-13556.416385	-13556.25552	-13556.32802	-13556.32777	
	2.009	-13556.383631	-	-	-	
TS- βH^{C}	0.0	-13556.399861	-13556.24238	-13556.31407	-13556.31362	-706.5605
	2.019	-13556.372177	-	-	-	
P βH^{C}	0.0	-13556.416196	-13556.25712	-13556.32910	-13556.32887	
	2.007	-13556.392402	-	-	-	

Table S6. SCF (E), enthalpies (H), and Gibbs free energies (G) and imaginary frequencies of the optimized intermediates and transition state structures for Ni-MFU-4l complex in toluene.

T(298K) solv				
A/B/C	<S ² >	E (a.u.)	H (a.u.)	G (a.u.)
AE1	2.008	-14371.954730	-14371.851757	-14371.921567
I1	0.0	-14450.387749	-14450.228125	-14450.304319
TS-I1	0.0	-14450.350232	-14450.193978	-14450.269111
P1	2.008	-14450.426327	-14450.265353	-14450.340086
I2	0.0	-14528.835985	-14528.607754	-14528.715043
TS-I2	0.0	-14528.815084	-14528.577689	-14528.683942
P2	2.008	-14528.893234	-14528.674199	-14528.753477
β H ^A	0.0	-14528.889285	-14528.670507	-14528.747608
TS- β H ^A	2.008	-14528.863712	-14528.650344	-14528.729389
P β H ^A	0.0	-14528.886318	-14528.669351	-14528.746868
AE2	2.008	-14293.553909	-14293.492835	-14293.532372
RI	0.0	-14371.960277	-14371.858914	-14371.924902
TS-RI	2.013	-14371.940289	-14371.842808	-14371.907794
β H ^B	0.0	-14450.423108	-14450.262403	-14450.334653
TS- β H ^B	0.0	-14450.411534	-14450.253910	-14450.325465
P β H ^B	0.0	-14450.419001	-14450.259594	-14450.331175
TS-cw	0.0	-14450.407866	-14450.250300	-14450.322260
P-cw	2.008	-14450.4185120	-14450.267877	-14450.342914
β H ^C	0.0	-14450.4254690	-14450.264785	-14450.337679
TS- β H ^C	0.0	-14450.403852	-14450.246464	-14450.317847
P β H ^C	0.0	-14450.4185020	-14450.257847	-14450.330232

Table S7. SCF (*E*), enthalpies (*H*), and Gibbs free energies (*G*) and imaginary frequencies of the optimized intermediates and transition state structures for Ni-CFA-1 complex in toluene.

T(298K)solv				
A/B/C	<S ² >	E (a.u.)	H (a.u.)	G (a.u.)
AE1	2.008	-13478.04046	-13477.94766	-13478.00655
I1	0.0	-13556.45442	-13556.32455	-13556.38649
TS-I1	0.0	-13556.40579	-13556.28694	-13556.35062
P1	2.008	-13556.50329	-13556.34257	-13556.41682
I2	0.0	-13634.93824	-13634.72010	-13634.79717
TS-I2	0.0	-13634.90798	-13634.69059	-13634.76061
P2	2.003	-13634.9696	-13634.75062	-13634.82987
β H ^A	0.0	-13634.97551	-13634.75688	-13634.83435
TS- β H ^A	0.0	-13634.96033	-13634.74504	-13634.82180
P β H ^A	0.0	-13634.96353	-13634.74649	-13634.82353

AE2	2.008	-13399.57453	-13399.55528	-13399.61506
RI	0.0	-13478.04423	-13477.94291	-13478.00872
TS-RI	2.008	-13478.02905	-13477.93177	-13477.99031
βH^{B}	0.0	-13556.5084	-13556.34784	-13556.42020
TS- βH^{B}	0.0	-13556.49563	-13556.33819	-13556.40950
P βH^{B}	0.0	-13556.49903	-13556.33975	-13556.41110
TS-cw	0.0	-13556.48781	-13556.33074	-13556.40224
P-cw	2.008	-13556.50725	-13556.34682	-13556.42166
βH^{C}	0.0	-13556.50544	-13556.34458	-13556.41683
TS- βH^{C}	0.0	-13556.4887	-13556.33122	-13556.40245
P βH^{C}	0.0	-13556.50377	-13556.34469	-13556.41644

Cartesian coordinates of the optimized structures

AE1

Ni-MFU-4l

Zn 21.50293300 9.70221700 5.72472800
 Cl 20.27476000 11.05873800 4.50824700
 Zn 23.49165400 7.51011500 7.74722300
 N 22.83036700 10.46847800 7.05846700
 C 23.07026900 11.75977000 7.41821600
 N 23.61475600 9.68346300 7.79709900
 C 22.50764600 12.96892800 6.96022800
 C 22.96920700 14.12420800 7.55716600
 H 21.74104900 12.99888800 6.17282200
 Zn 21.35570100 5.51865000 9.81737600
 Cl 20.04384200 4.31447500 11.10291500
 N 20.51781600 6.85259200 8.53026100
 C 19.22204900 7.17839100 8.25686600
 N 21.30324000 7.60677400 7.76522400
 C 18.00417800 6.69434900 8.77684700
 C 16.85322900 7.25964200 8.26382200
 H 17.96050500 5.91262000 9.54800300
 Ni 25.67822700 9.49593400 9.85323600
 N 24.29133200 8.30383600 10.68331500
 C 23.89813900 8.12376800 11.98140400
 N 23.55000300 7.50037300 9.92451900
 C 24.30514200 8.71938100 13.19431800
 C 23.66818800 8.29483600 14.34224100
 N 20.57839000 8.41516600 6.99656800
 C 19.26194000 8.18663600 7.26594000
 C 18.08551700 8.76261900 6.74429400
 C 16.89590200 8.28541000 7.25570300
 H 18.10351600 9.54843400 5.97620500
 N 24.36635800 10.40051600 8.62844400
 C 24.05862800 11.71834300 8.43011000
 C 24.51854200 12.90587700 9.03820500

C	23.96623900	14.08811500	8.59007300
H	25.26982800	12.91608300	9.83597400
N	22.69421800	6.79449900	10.66312800
C	22.87205500	7.14946500	11.96614000
C	22.22300600	6.71446500	13.13991800
C	22.63570100	7.29731400	14.32053100
H	21.42890300	5.95432500	13.12397000
N	22.59209200	4.59166800	8.49886100
C	22.81067400	3.27539100	8.21675600
N	23.37958900	5.31888300	7.71103400
C	22.24819000	2.09732900	8.74910700
C	22.70901200	0.90714600	8.22129100
H	21.48487800	2.11220100	9.53959200
Zn	25.43281500	5.36474700	5.61484600
Cl	26.63883500	4.06272600	4.31984700
N	24.18667300	6.73536700	4.77310500
C	23.92065000	7.04919400	3.47264900
N	23.45779100	7.53499000	5.54719700
C	24.41251300	6.52031600	2.26194600
C	23.91675500	7.08555800	1.10451000
N	24.11037600	4.53679600	6.92072000
C	23.79137500	3.23996100	7.19838600
C	24.26033700	2.02358700	6.66168400
C	23.70719800	0.87289600	7.18607600
H	25.02248500	1.98182400	5.87106200
N	22.72218300	8.36319400	4.81038200
C	22.97422900	8.09948300	3.49645300
C	22.47032700	8.67369100	2.31170400
C	22.95341500	8.15354800	1.12686300
H	21.73427500	9.48968800	2.31727900
N	26.36205400	6.61285300	6.92392700
C	27.67316400	6.84784800	7.20643400
N	25.63183500	7.39723000	7.71390100
C	28.85202500	6.29357600	6.66790900
C	30.04293600	6.76223900	7.18626100
H	28.83583000	5.52940700	5.87812500
N	26.39567000	8.13872200	8.50509100
C	27.69895800	7.83011300	8.22371500
C	28.91994800	8.30338700	8.74732000
C	30.07404600	7.76043800	8.21905300
H	28.98051600	9.06178500	9.53921200
H	25.14866300	5.70495700	2.22972900
C	22.94931300	8.18950900	-1.23687400
C	23.90367900	7.13182000	-1.25786400
C	22.46152200	8.74582800	-2.40479100
C	24.39138800	6.60711200	-2.44529200
C	22.94559200	8.22540500	-3.61869400
C	23.89219400	7.17623800	-3.62692600
H	25.12640100	5.79202900	-2.41473100
C	32.40523700	6.69519700	7.18989900
C	32.43545500	7.68502300	8.21430400

C	33.56874800	6.15706300	6.67184600
C	33.62689900	8.15816000	8.74314600
C	34.78660000	6.62586800	7.19666900
C	34.80383500	7.60773600	8.21277500
H	33.60380100	8.92152800	9.53199000
C	14.53479100	8.37608900	7.25721100
C	14.49124800	7.36049000	8.25542100
C	13.38160500	8.94800800	6.74131300
C	13.29146100	6.89425900	8.76001100
C	12.16734800	8.47028700	7.25766600
C	12.11150500	7.46350800	8.24774100
H	13.27647100	6.11103400	9.52904600
C	22.62620500	-1.45544100	8.20947500
C	23.61510000	-1.48820900	7.18428900
C	22.08235100	-2.61689500	8.72595700
C	24.08210700	-2.68101200	6.65300000
C	22.54478400	-3.83616700	8.19834400
C	23.52600000	-3.85599800	7.18165100
H	24.84526500	-2.65943300	5.86390900
O	31.20633800	6.24443100	6.68413000
O	31.27103800	8.21052700	8.71871800
H	33.52734000	5.39510000	5.88269600
N	36.08945900	6.28414300	6.88622500
N	36.14134600	7.78728500	8.44266400
N	36.88968900	6.98000200	7.63240100
O	22.18234500	-0.25434100	8.71721300
O	24.14514000	-0.32574300	6.68201600
H	21.32115200	-2.57314400	9.51573900
N	22.19710900	-5.13802100	8.50642300
N	23.69911900	-5.19385400	6.94901300
N	22.88881300	-5.94006600	7.75819500
C	23.44001900	8.47085200	16.68741300
C	22.41801300	7.47778800	16.66612600
C	23.85456200	9.07143500	17.86687100
C	21.78898000	7.06416600	17.82589700
C	23.21191900	8.64694400	19.03993200
C	22.19769400	7.66308100	19.03126300
H	21.00360400	6.29796300	17.79095500
O	22.02646600	6.89895700	15.47955600
O	24.05612100	8.87093700	15.52765400
H	24.64548800	9.83244300	17.83754200
N	23.31428800	8.96980100	20.36636200
N	21.76317000	7.46078200	20.32779500
N	22.43279400	8.24240300	21.11643500
H	25.08022400	9.49077200	13.25115400
O	22.48348600	8.68994500	-0.04106500
O	24.37800100	6.59024600	-0.08914800
H	21.72641800	9.56036900	-2.36995600
N	24.10103100	6.96258800	-4.96286200
N	23.34325800	7.81262900	-5.71868500
N	22.65118900	8.56917600	-4.92472500

O	15.65465300	6.81147600	8.74817600
H	13.46193900	9.72803600	5.97277800
O	15.73461300	8.82792100	6.76666400
N	10.84683600	8.75233500	7.03272700
N	10.78672400	7.20921800	8.54925800
N	10.04042300	7.98076100	7.82163900
C	22.88271100	16.47920700	7.72879700
C	23.86991900	16.44341800	8.75615400
C	22.33577700	17.67257900	7.29454600
C	24.33057000	17.59824300	9.37099000
C	22.79221900	18.85353200	7.90743300
C	23.77113300	18.80559700	8.92534000
H	25.09208600	17.52477200	10.15855200
O	22.44390700	15.31624300	7.13640200
O	24.40487300	15.25104900	9.17602000
H	21.57635600	17.68156300	6.50189800
N	22.43972400	20.17247700	7.69104100
N	23.12637400	20.92269800	8.49548400
N	23.93818700	20.12449500	9.25208800
H	23.92816200	9.64230500	20.82708400
H	10.42533500	9.42386700	6.39014500
H	24.31877800	-5.66459800	6.28877800
H	36.61087400	8.40921800	9.10163200
H	24.55417400	20.55031200	9.94535600
H	24.71326500	6.29036000	-5.42631500
C	26.30274400	10.82115400	11.17927400
H	26.72314100	11.65402500	10.56739400
H	25.47427000	11.25231900	11.78087200
C	27.41250600	10.23653800	12.06820500
H	28.29245300	9.90614100	11.47536800
H	27.80152300	10.97123500	12.81207500
H	27.08309500	9.34927800	12.65032100

Ni-CFA-1

Zn	-0.59380700	2.97118000	-2.72285300
Cl	-0.88602600	4.56562800	-4.20359100
Zn	-0.07423600	0.34324800	-0.32611400
N	1.28452900	2.42888600	-2.16836000
C	2.49644900	2.87993500	-2.60195100
N	1.50251200	1.47239000	-1.26735100
C	2.85188200	3.86535800	-3.54680000
C	4.20342000	4.06145200	-3.75323200
H	2.07881400	4.44318400	-4.07455200
Zn	-1.70421400	1.22581600	2.75318100
Cl	-2.68481600	1.77241000	4.64348100
N	-1.82058200	2.49539900	1.17532400
C	-2.41947400	3.71515300	1.03258000
N	-1.22179300	2.19326200	0.02809800
C	-3.18462800	4.48691500	1.92618700
C	-3.66459900	5.70980900	1.46306000

H	-3.40361000	4.10889400	2.93551900
Ni	3.48146400	-0.11544800	0.25339700
N	2.22123400	0.35503800	1.78166700
C	2.44521500	0.48973800	3.13081800
N	0.92919000	0.58079900	1.57336700
C	3.60530000	0.33125400	3.91423800
C	3.49245900	0.52403100	5.28822500
N	-1.39855800	3.15918100	-0.86728000
C	-2.14702800	4.14213200	-0.28669300
C	-2.62641400	5.37909200	-0.76568500
C	-3.37045700	6.13409700	0.12088500
H	-2.40149500	5.71547400	-1.78827500
N	2.80087700	1.26915900	-1.07503500
C	3.47390900	2.13614800	-1.90138900
C	4.84769000	2.33432200	-2.13961000
C	5.21348600	3.30929900	-3.06293600
H	5.60174700	1.72247300	-1.62992700
N	0.29394800	0.87082300	2.70793300
C	1.20480700	0.82434200	3.72181300
C	1.07735000	1.02927900	5.11156500
C	2.22518400	0.87651100	5.86431900
H	0.10309200	1.28115500	5.55582800
N	-2.29222400	-0.45994200	1.77614900
C	-3.25952000	-1.38545600	2.04098300
N	-1.69541700	-0.80260900	0.63937300
C	-4.18412400	-1.51547600	3.09796100
C	-5.03695300	-2.60112900	3.03656000
H	-4.20397400	-0.78994700	3.92422300
Zn	-1.51982700	-2.71090800	-1.58999800
Cl	-2.43166000	-4.56048900	-2.35559900
N	-1.60771900	-1.02231600	-2.71540400
C	-2.16177400	-0.78116400	-3.94021700
N	-1.10030100	0.11891800	-2.26179100
C	-2.81708000	-1.63271500	-4.84803200
C	-3.27538700	-1.06699900	-6.03552200
N	-2.22520500	-1.91505600	0.14194800
C	-3.21617800	-2.32637400	0.98754400
C	-4.09160200	-3.42651500	0.93054400
C	-5.01300900	-3.56134700	1.96661900
H	-4.05105400	-4.12405000	0.08114900
N	-1.29184900	1.10337600	-3.13363400
C	-1.95671500	0.59078400	-4.21000100
C	-2.41494600	1.17377300	-5.40989200
C	-3.06492200	0.33199300	-6.29273600
H	-2.26343100	2.24415500	-5.61198000
N	0.45756300	-2.63904600	-1.14887800
C	1.44264600	-3.57582000	-1.25229700
N	1.00852800	-1.51712700	-0.68710000
C	1.42664200	-4.91928300	-1.68059600
C	2.63604900	-5.58701400	-1.65724600
H	0.49039300	-5.39836100	-2.00263800

N	2.31037800	-1.66298300	-0.47820600
C	2.63677200	-2.95496900	-0.82037200
C	3.86296700	-3.64644700	-0.80313800
C	3.86219100	-4.97332200	-1.22745800
H	4.78970900	-3.14324200	-0.49114700
H	-2.93046900	-2.70298700	-4.62162000
H	4.56792000	0.08080600	3.45186600
C	-4.48404300	6.57963600	2.34985900
C	-4.19026500	6.64600100	3.74666800
C	-5.54718700	7.32527400	1.83494100
C	-4.92018500	7.42274800	4.63440300
H	-3.33608900	6.06771800	4.12891000
C	-6.29728900	8.11647700	2.71814500
H	-5.82317500	7.28585000	0.77192900
C	-5.98613600	8.16065500	4.09515500
H	-4.66243600	7.45742300	5.70243200
H	-7.07331400	9.33913900	5.55431500
C	6.65308900	3.58308000	-3.32048400
C	7.10653900	3.85234900	-4.64730100
C	7.57030200	3.57291200	-2.26641000
C	8.43656900	4.10651000	-4.95179400
H	6.37102600	3.83359900	-5.46535800
C	8.91916100	3.82858600	-2.55521000
H	7.25463400	3.39584400	-1.22825300
C	9.34074200	4.09172200	-3.87788000
H	8.75609500	4.29990300	-5.98568500
H	11.39193300	4.50804100	-4.44416700
C	4.68377300	0.35535500	6.16385700
C	4.91271300	1.26272900	7.24228300
C	6.01092300	1.16853300	8.08571900
H	4.19877600	2.08620400	7.39302300
C	5.58985000	-0.68188000	5.93216200
C	6.90819300	0.11835400	7.83443500
H	6.16544600	1.89040100	8.90023100
C	6.70524700	-0.79438000	6.77538300
H	5.43373600	-1.41524600	5.12856600
C	-5.97697700	-4.69487000	1.96735700
C	-5.56030700	-5.97979100	1.50155100
C	-6.41632200	-7.06855400	1.46480800
H	-4.51572700	-6.10446400	1.18096900
C	-7.29038900	-4.50249000	2.41019700
C	-7.73682000	-6.87639800	1.90653700
H	-6.08512000	-8.05541500	1.11248500
C	-8.15133700	-5.60757300	2.36986900
H	-7.63546800	-3.51396400	2.74511300
H	10.15625000	-5.16347600	3.06883300
C	-3.98679700	-1.90785900	-7.03599700
C	-3.77442000	-1.69405500	-8.43236100
C	-4.40085900	-2.45867000	-9.40381700
H	-3.06648400	-0.91057600	-8.73986600
C	-4.85479200	-2.91784000	-6.60600700

C	-5.27284600	-3.47336500	-8.97366100
H	-4.22420200	-2.29429800	-10.47599200
C	-5.48341900	-3.68816300	-7.59292000
H	-5.04560400	-3.08003600	-5.53565600
H	-6.79672700	-5.21282800	-6.78482100
C	5.12584200	-5.75879600	-1.24330800
C	6.06864600	-5.60898800	-0.18080900
C	7.26761000	-6.30327800	-0.14950500
H	5.81345400	-4.93623300	0.65112300
C	5.39410500	-6.63503900	-2.30068700
C	7.54095600	-7.18016600	-1.21321700
H	7.98339900	-6.18957900	0.67662400
C	6.60825000	-7.33394300	-2.26370100
H	4.69030000	-6.74202800	-3.13837400
H	6.90118800	-8.64252700	-3.96856900
N	8.63236600	-7.99315900	-1.46327500
N	8.43234500	-8.62104600	-2.57930400
N	7.22138000	-8.24211000	-3.08611000
N	-6.37511000	-4.72827100	-7.57813400
N	-6.68287300	-5.12632300	-8.84763800
N	-6.03335900	-4.38230000	-9.68771100
N	11.06799300	4.15979000	-2.43155200
N	10.02176600	3.88812600	-1.71790000
N	10.68805100	4.29000700	-3.73805200
N	-7.39052800	8.93498300	2.48345000
N	-7.75536300	9.46859000	3.60603500
N	-6.92697000	9.01937300	4.59625100
N	-8.80619800	-7.75094200	1.98390700
N	-9.83028200	-7.11032200	2.45437400
N	-9.46642300	-5.81546700	2.69387500
N	7.73997200	-1.71588900	6.77878400
N	8.54745300	-1.42601600	7.74929300
N	8.07093500	-0.32560900	8.40470100
H	8.58792900	0.04322000	9.20365000
H	-5.75526000	-2.75851300	3.85461800
H	4.52742700	4.83976600	-4.45987900
H	2.66671800	-6.64521200	-1.95594900
H	2.16793900	0.99944700	6.95599800
H	-3.46209700	0.75017500	-7.22924100
H	-3.74134800	7.11808100	-0.20157500
C	5.27029100	0.52165300	0.82110900
H	5.60778100	-0.19032300	1.61121600
H	5.93864700	0.34630400	-0.05504300
C	5.33184500	1.97276300	1.30200700
H	4.68751400	2.13978900	2.18928300
H	6.35960100	2.29326000	1.59013900
H	4.98298900	2.68064600	0.52230200

II

Ni-MFU-4l

Zn	21.47823600	9.71980100	5.80777700
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Cl	20.26990600	11.09013300	4.58606700
Zn	23.45680400	7.48382400	7.83712200
N	22.76075800	10.48489900	7.18288300
C	23.07265500	11.77616600	7.49290700
N	23.46726800	9.68804400	7.98901300
C	22.52660300	12.99033100	7.03653200
C	23.01084000	14.13590800	7.62817900
H	21.74879700	13.03025000	6.26060900
Zn	21.30533200	5.49811100	9.88527900
Cl	19.96320400	4.27503100	11.11863100
N	20.49442700	6.85075000	8.59093600
C	19.20162400	7.19017400	8.32468700
N	21.28016600	7.59861700	7.82224500
C	17.98644600	6.70297700	8.84088300
C	16.83926300	7.27125500	8.33041000
H	17.94289900	5.91465800	9.60544900
Ni	25.62786000	9.40273900	9.91922900
N	24.24712800	8.22672400	10.72166900
C	23.87063600	8.13742900	12.04434300
N	23.50185500	7.41722300	9.99458900
C	24.27426000	8.74416900	13.25006800
C	23.63918500	8.32346600	14.39704100
N	20.55824500	8.41690700	7.06151100
C	19.24206200	8.20157800	7.34217000
C	18.06897100	8.78018700	6.82300200
C	16.88243300	8.29986700	7.33101300
H	18.08654500	9.56821300	6.05727700
N	24.22070000	10.39687800	8.81753000
C	24.06433200	11.72297200	8.49627400
C	24.54806500	12.90050000	9.09927500
C	24.01116000	14.08688200	8.65210900
H	25.25963400	12.91274700	9.93235500
N	22.64387700	6.75087700	10.75680500
C	22.85035600	7.16164300	12.03427700
C	22.20408700	6.73086300	13.20796500
C	22.61511400	7.32259500	14.38152600
H	21.41031400	5.97072800	13.19850700
N	22.54511300	4.60000700	8.54246600
C	22.79559900	3.28686400	8.27980100
N	23.31106800	5.32914600	7.73749400
C	22.23667400	2.10936300	8.81005400
C	22.70120500	0.92487000	8.28016600
H	21.46868200	2.12096300	9.59611900
Zn	25.41367900	5.37230600	5.67369300
Cl	26.57928400	4.07479600	4.33696400
N	24.18966200	6.77917900	4.84690400
C	23.89670000	7.07743500	3.54703300
N	23.47850000	7.59009500	5.62613900
C	24.38841300	6.55259100	2.33748000
C	23.89435100	7.12328400	1.18537800
N	24.06009300	4.55356700	6.95965800

C	23.77406000	3.25605400	7.26409500
C	24.24649700	2.04503500	6.72533200
C	23.69672700	0.89528400	7.24786400
H	25.00385400	2.00694900	5.92993900
N	22.72753700	8.40885700	4.89142700
C	22.95416200	8.12645400	3.57422900
C	22.45218200	8.70606900	2.39435100
C	22.93538000	8.18966300	1.21132800
H	21.72049900	9.52593600	2.40274900
N	26.34741400	6.54641100	7.03054800
C	27.64687000	6.88181000	7.27580200
N	25.60172100	7.18874300	7.93269500
C	28.82838200	6.34139700	6.73587500
C	30.01136100	6.82373700	7.25259300
H	28.82104200	5.56974500	5.95340400
N	26.35836600	7.91388100	8.73959600
C	27.66413300	7.86220600	8.29059200
C	28.87768800	8.35036500	8.81193200
C	30.03334000	7.82023700	8.28191500
H	28.96146700	9.03960100	9.65387600
H	25.12556200	5.73808200	2.30376100
C	22.93429400	8.23582800	-1.15366000
C	23.88412100	7.17991500	-1.17815200
C	22.44919700	8.79852900	-2.31631300
C	24.37359600	6.65923300	-2.36309300
C	22.93420600	8.28321000	-3.52957100
C	23.87717600	7.23470900	-3.54004100
H	25.10722500	5.84293300	-2.33465300
C	32.37570300	6.78346000	7.25217800
C	32.39677400	7.77172600	8.27230600
C	33.54062900	6.25738900	6.73248900
C	33.57973900	8.25923400	8.79916800
C	34.75185100	6.73997700	7.25439600
C	34.75891600	7.72116800	8.26722800
H	33.54963600	9.02148600	9.58875800
C	14.52001200	8.39130200	7.33219900
C	14.47598100	7.37323600	8.32165000
C	13.37144700	8.96756900	6.81900600
C	13.27935900	6.90485400	8.82400900
C	12.15966400	8.48772000	7.33290000
C	12.10209000	7.47761300	8.31530900
H	13.26431100	6.11724600	9.58849600
C	22.62520900	-1.43928500	8.26393000
C	23.61119600	-1.46741200	7.24183200
C	22.08444900	-2.59974300	8.77841100
C	24.08224000	-2.65378200	6.70759800
C	22.55007100	-3.81441700	8.24873100
C	23.52936100	-3.82846800	7.23410100
H	24.84505200	-2.62808800	5.91841000
O	31.18192200	6.31578900	6.75131700
O	31.22629100	8.27840400	8.78524700

H	33.50542700	5.49333700	5.94515400
N	36.05840500	6.41182500	6.94228500
N	36.09501900	7.91676900	8.49641900
N	36.85166800	7.11721600	7.68686700
O	22.17709400	-0.24011000	8.77303900
O	24.13717100	-0.30208700	6.74104100
H	21.32291700	-2.55907600	9.56797600
N	22.20570900	-5.11833700	8.55436900
N	23.70743600	-5.16561000	6.99737300
N	22.89981200	-5.91651900	7.80432700
C	23.40611800	8.51640700	16.74190400
C	22.39377700	7.51955100	16.72690200
C	23.81545700	9.12978600	17.91298300
C	21.76530900	7.11106100	17.88543400
C	23.17351700	8.71059400	19.08554900
C	22.16776700	7.72216600	19.08425800
H	20.98421100	6.34048100	17.85407400
O	22.00278100	6.93052300	15.54516300
O	24.01370600	8.92231600	15.57754800
H	24.59926100	9.89780600	17.87844900
N	23.27243200	9.04682800	20.40971600
N	21.73157100	7.52817900	20.38220600
N	22.39444500	8.32120700	21.16506500
H	24.93094100	9.54954400	13.50030200
O	22.46804000	8.73187100	0.04446600
O	24.35608000	6.63279200	-0.01053300
H	21.71545600	9.61412800	-2.27858800
N	24.08924500	7.02558700	-4.87680000
N	23.33485000	7.87974900	-5.63069500
N	22.64243700	8.63391700	-4.83492400
O	15.63928000	6.82009800	8.81067600
H	13.45273600	9.75164900	6.05482200
O	15.72077800	8.84464800	6.84389500
N	10.83925700	8.77353800	7.10825500
N	10.77660100	7.22261800	8.61571200
N	10.03144300	7.99891900	7.89214400
C	22.96112600	16.49371900	7.79657100
C	23.95109600	16.44509500	8.81469600
C	22.42837000	17.69080400	7.36390500
C	24.43278300	17.58974600	9.42554900
C	22.90534600	18.86351500	7.97206900
C	23.88788500	18.80168800	8.98164700
H	25.19684000	17.50631500	10.20955500
O	22.49970000	15.33518300	7.21096000
O	24.46653600	15.24362000	9.23740000
H	21.66347500	17.70937900	6.57673600
N	22.56985600	20.18753100	7.75645500
N	23.27221000	20.92791000	8.55608800
N	24.07692400	20.11839800	9.30752900
H	23.88137600	9.72761600	20.86458700
H	10.41962800	9.44923700	6.46887300

H	24.32881600	-5.63196200	6.33570100
H	36.55752700	8.54460900	9.15468300
H	24.70348400	20.53502900	9.99693400
H	24.70136000	6.35383300	-5.34107500
C	25.46666000	10.19343100	11.69220800
H	24.41182400	10.24938300	11.95549800
C	26.55715600	9.57934500	12.59388900
H	27.54837700	9.85644600	12.17024200
H	26.58187700	9.97186700	13.63702000
H	26.54656600	8.47302800	12.66391700
C	26.82965400	10.09741200	8.33141500
H	27.57514200	9.63925200	7.69419100
C	27.18155700	10.74618800	9.50915400
H	26.70708600	11.68794100	9.80427400
H	28.11545400	10.53717000	10.04894000
H	26.06824600	10.58538600	7.70640400
H	25.75094100	11.26762200	11.59388500

Ni-CFA-1

Zn	-0.76126600	2.89458300	-2.75762200
Cl	-1.06482700	4.48918000	-4.23565300
Zn	-0.22980500	0.28439700	-0.39340200
N	1.11951700	2.36235600	-2.20401500
C	2.33628000	2.79587200	-2.62970600
N	1.33277100	1.41385800	-1.29566900
C	2.69171000	3.78123900	-3.57463200
C	4.04324000	3.97736600	-3.78105600
H	1.91935500	4.35999000	-4.10248300
Zn	-1.86582800	1.14547600	2.72424700
Cl	-2.85332700	1.67245900	4.61771000
N	-1.99962200	2.40129800	1.13907900
C	-2.57968400	3.63101700	1.00474700
N	-1.40834400	2.09756700	-0.01123400
C	-3.34478200	4.40283200	1.89838400
C	-3.82477500	5.62571600	1.43524000
H	-3.56678400	4.02367300	2.90671300
Ni	3.31056200	-0.14663600	0.23814700
N	2.09599500	0.52549900	1.74163400
C	2.28503500	0.40562600	3.10305600
N	0.80443800	0.72931400	1.52791900
C	3.44516600	0.24712800	3.88640200
C	3.33223900	0.43995300	5.26039800
N	-1.57229000	3.06955900	-0.90097500
C	-2.30719300	4.05801500	-0.31449400
C	-2.78657800	5.29500500	-0.79350900
C	-3.53063800	6.05000100	0.09306700
H	-2.56351800	5.63031000	-1.81695700
N	2.62641100	1.20550800	-1.10191100
C	3.31374400	2.05206500	-1.92922500
C	4.68753000	2.25019200	-2.16741800
C	5.05329000	3.22520400	-3.09076100

H	5.45739000	1.65080500	-1.67852700
N	0.14478200	0.87948600	2.67892800
C	1.04461900	0.74034000	3.69389800
C	0.91718700	0.94512300	5.08374300
C	2.06498600	0.79236300	5.83652600
H	-0.05171600	1.22375200	5.52408600
N	-2.41945500	-0.56794600	1.77046000
C	-3.41970100	-1.46952500	2.01314800
N	-1.80258600	-0.92627500	0.64662900
C	-4.34428800	-1.59959800	3.07015100
C	-5.19714300	-2.68521400	3.00873400
H	-4.36029000	-0.87703700	3.89918500
Zn	-1.68385000	-2.80018300	-1.62611400
Cl	-2.64415900	-4.63715300	-2.36625000
N	-1.80284300	-1.09508400	-2.72647800
C	-2.32194600	-0.86525500	-3.96796400
N	-1.31054000	0.05067700	-2.26971200
C	-2.97722600	-1.71682300	-4.87586700
C	-3.43556400	-1.15109000	-6.06334100
N	-2.35323800	-2.02395800	0.13613900
C	-3.37634000	-2.41045200	0.95970800
C	-4.25175500	-3.51063200	0.90274700
C	-5.17318800	-3.64544400	1.93880200
H	-4.20731800	-4.21020600	0.05505700
N	-1.47888600	1.02870600	-3.15178600
C	-2.11688600	0.50667300	-4.23777800
C	-2.57511400	1.08968300	-5.43771400
C	-3.22509700	0.24789800	-6.32055800
H	-2.42709300	2.16093500	-5.63818000
N	0.30184100	-2.70573500	-1.30061500
C	1.28237200	-3.65968900	-1.27997400
N	0.88860300	-1.53021500	-1.05223700
C	1.26653300	-5.00334800	-1.70844300
C	2.47585400	-5.67114200	-1.68503600
H	0.33392700	-5.47876900	-2.04685100
N	2.19307300	-1.67300700	-0.88365400
C	2.47657400	-3.03950400	-0.84837900
C	3.70294900	-3.73042000	-0.83088700
C	3.70190900	-5.05741800	-1.25528800
H	4.64053200	-3.21825700	-0.57485400
H	-3.09605900	-2.78598600	-4.64668200
H	4.45611900	0.29508600	3.47480700
C	-4.64422600	6.49554200	2.32203800
C	-4.35044700	6.56190500	3.71884900
C	-5.70736900	7.24117800	1.80712200
C	-5.08036500	7.33865400	4.60658400
H	-3.49610900	5.98367700	4.10098200
C	-6.45746900	8.03238300	2.69032600
H	-5.98327100	7.20167300	0.74403500
C	-6.14631600	8.07656200	4.06733500
H	-4.82261300	7.37338300	5.67468000

H	-7.23349200	9.25541800	5.52644600
C	6.49291000	3.49898200	-3.34829900
C	6.94635800	3.76826000	-4.67511900
C	7.41012100	3.48882300	-2.29422800
C	8.27638900	4.02241600	-4.97961400
H	6.21054000	3.74956700	-5.49295000
C	8.75898000	3.74449200	-2.58303000
H	7.09328600	3.31319900	-1.25632600
C	9.18056200	4.00762600	-3.90569900
H	8.59598100	4.21600900	-6.01353100
H	11.23200000	4.42393900	-4.47180800
C	4.52359500	0.27126800	6.13603600
C	4.75253600	1.17863700	7.21446100
C	5.85074200	1.08443900	8.05790000
H	4.03918500	2.00269400	7.36502200
C	5.42967200	-0.76597200	5.90433800
C	6.74801000	0.03425900	7.80661900
H	6.00534400	1.80650600	8.87227400
C	6.54506600	-0.87847600	6.74756500
H	5.27050600	-1.50087700	5.10209200
C	-6.13716100	-4.77896100	1.93953700
C	-5.72048800	-6.06388400	1.47372800
C	-6.57650200	-7.15264800	1.43699000
H	-4.67611500	-6.18851200	1.15226700
C	-7.45057000	-4.58658300	2.38237500
C	-7.89700000	-6.96049200	1.87871900
H	-6.24519900	-8.13942800	1.08436600
C	-8.31151700	-5.69166700	2.34205100
H	-7.79573300	-3.59800600	2.71727800
H	10.31661700	-5.24757000	3.04088800
C	-4.14697700	-1.99195700	-7.06381300
C	-3.93460300	-1.77814600	-8.46018000
C	-4.56103900	-2.54276400	-9.43163700
H	-3.22657400	-0.99463900	-8.76758900
C	-5.01497500	-3.00193200	-6.63382600
C	-5.43302600	-3.55745900	-9.00148000
H	-4.38417000	-2.37838100	-10.50383900
C	-5.64359900	-3.77225700	-7.62073900
H	-5.20551400	-3.16449300	-5.56340900
H	-6.95646500	-5.29737800	-6.81260100
C	4.96567600	-5.84286600	-1.27114600
C	5.90846400	-5.69308200	-0.20862500
C	7.10742700	-6.38737600	-0.17732300
H	5.65210400	-5.02036300	0.62338100
C	5.23392500	-6.71913500	-2.32850300
C	7.38077500	-7.26426000	-1.24103600
H	7.82316400	-6.27416400	0.64901900
C	6.44806700	-7.41804100	-2.29151800
H	4.53008100	-6.82541100	-3.16627500
H	6.74150400	-8.72629000	-3.99669300
N	8.47220800	-8.07742300	-1.49108900

N	8.27263200	-8.70474500	-2.60742100
N	7.06157200	-8.32611000	-3.11400300
N	-6.53512700	-4.81273100	-7.60604800
N	-6.84383700	-5.21016400	-8.87547900
N	-6.19328700	-4.46706000	-9.71540500
N	10.90811300	4.07661300	-2.45926000
N	9.86193500	3.80378700	-1.74583500
N	10.52818900	4.20585200	-3.76560600
N	-7.55074100	8.85122200	2.45580900
N	-7.91609700	9.38419200	3.57840700
N	-7.08722900	8.93554800	4.56836300
N	-8.96659600	-7.83503700	1.95649200
N	-9.99084200	-7.19429100	2.42611000
N	-9.62671200	-5.89969900	2.66618300
N	7.58002000	-1.79963600	6.75046200
N	8.38722500	-1.51023800	7.72126300
N	7.91098300	-0.40975800	8.37637800
H	8.42799500	-0.04121400	9.17561300
H	-5.91369600	-2.84377500	3.82820700
H	4.36661600	4.75641200	-4.48754000
H	2.50897100	-6.72692200	-1.99210200
H	2.00915600	0.92538800	6.92732400
H	-3.62436700	0.66650300	-7.25608400
H	-3.90268200	7.03345600	-0.22989800
C	5.07634900	0.69509800	0.57093300
H	5.72490500	0.09184000	1.23664900
H	5.50957300	0.53138400	-0.44081000
C	5.13780800	2.14622600	1.05208800
H	4.76821200	2.22964800	2.09559700
H	6.17705500	2.54880700	1.05187400
H	4.51851700	2.83614200	0.44331600
C	4.09549600	-1.60754600	1.79965000
H	4.32320500	-0.93696700	2.60862000
H	4.95484500	-2.21653200	1.46135900
C	2.87959100	-1.83644500	1.18864100
H	2.82391500	-2.86913800	0.88035600
H	1.93499900	-1.57855900	1.68548300

TS-II

Ni-MFU-4l

Zn	21.49960220	9.69219977	5.83251282
Cl	20.27224320	11.04624277	4.61038782
Zn	23.46933120	7.52426677	7.82913082
N	22.81159720	10.48999377	7.13945782
C	23.07206820	11.77406877	7.49746482
N	23.59206320	9.69839877	7.87001682
C	22.52614120	12.98821377	7.04099682
C	23.01034320	14.13378877	7.63267482
H	21.76569720	13.02916277	6.26859982
Zn	21.34368020	5.55226977	9.87248882

Cl	20.03402920	4.33492077	11.14602282
N	20.49289620	6.86130377	8.60223082
C	19.20111220	7.18799677	8.32912782
N	21.27628920	7.61802377	7.84275782
C	17.98594720	6.70088277	8.84540982
C	16.83876320	7.26913977	8.33491482
H	17.94295120	5.92477077	9.60175182
Ni	25.66320120	9.48883577	9.92171082
N	24.26593820	8.30510177	10.75362382
C	23.86985720	8.13554977	12.04891582
N	23.52371620	7.49931277	10.00248182
C	24.27387720	8.74196777	13.25457982
C	23.63868820	8.32132777	14.40153682
N	20.55484320	8.42954177	7.07911982
C	19.24154520	8.19948877	7.34668082
C	18.06846820	8.77806477	6.82750582
C	16.88193320	8.29774477	7.33551082
H	18.08729420	9.55705077	6.07314482
N	24.28679654	10.45384285	8.62469510
C	24.06373820	11.72086577	8.50081482
C	24.54760620	12.89837277	9.10375782
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H	25.29323920	12.89216477	9.88692282
N	22.66968120	6.79818777	10.74222882
C	22.84988420	7.15949677	12.03880682
C	22.20362620	6.72869277	13.21246482
C	22.61462520	7.32045577	14.38603082
H	21.42298420	5.97561577	13.20221082
N	22.57321320	4.59641077	8.56877182
C	22.79505320	3.28474577	8.28424282
N	23.35776420	5.32422877	7.78445182
C	22.23619720	2.10724477	8.81458282
C	22.70070920	0.92274977	8.28466982
H	21.48283120	2.11928877	9.59470882
Zn	25.39074320	5.40652777	5.71002182
Cl	26.61096720	4.11648077	4.41613382
N	24.16124320	6.75667877	4.84718382
C	23.89614720	7.07527277	3.55145382
N	23.43370820	7.55269677	5.62108982
C	24.38792220	6.55047477	2.34198182
C	23.89385320	7.12116477	1.18987782
N	24.08994220	4.54816577	6.99381982
C	23.77352720	3.25393977	7.26856782
C	24.24600320	2.04291377	6.72983982
C	23.69622820	0.89316377	7.25236482
H	24.99854520	2.00564577	5.94972582
N	22.70027620	8.38335577	4.89014182
C	22.95363520	8.12433777	3.57868382
C	22.45169820	8.70396277	2.39884982
C	22.93488220	8.18754377	1.21582782
H	21.72640220	9.51025977	2.40823182

N	26.33895020	6.63549277	7.00162482
C	27.64648920	6.87985377	7.28009582
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C	28.82786920	6.33925477	6.74037282
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H	28.81853320	5.58541977	5.96050482
N	26.36260920	8.15744277	8.58236382
C	27.66404720	7.85960077	8.29543182
C	28.87713020	8.34848477	8.81635882
C	30.03283720	7.81817377	8.28634882
H	28.92368320	9.10136777	9.59450282
H	25.11350320	5.74507777	2.30791982
C	22.93379120	8.23370577	-1.14916018
C	23.88361820	7.17779277	-1.17365218
C	22.44869920	8.79641077	-2.31181318
C	24.37309620	6.65711377	-2.35859318
C	22.93370720	8.28109077	-3.52507118
C	23.87667720	7.23258877	-3.53554118
H	25.09743020	5.85118777	-2.33491918
C	32.37520220	6.78131377	7.25670482
C	32.39627320	7.76957977	8.27683282
C	33.54012920	6.25526977	6.73698782
C	33.57923920	8.25711277	8.80366982
C	34.75135120	6.73786477	7.25888782
C	34.75841620	7.71905377	8.27172282
H	33.55327320	9.01126477	9.58172882
C	14.51951220	8.38917977	7.33669682
C	14.47548120	7.37111077	8.32614382
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C	13.27885920	6.90273277	8.82850782
C	12.15916420	8.48560177	7.33740182
C	12.10159020	7.47549377	8.31980982
H	13.26458520	6.12533377	9.58332682
C	22.62470620	-1.44140523	8.26842682
C	23.61069420	-1.46953223	7.24632882
C	22.08394920	-2.60186323	8.78291082
C	24.08174220	-2.65590223	6.71209982
C	22.54957120	-3.81653723	8.25323082
C	23.52886220	-3.83058823	7.23860182
H	24.83500120	-2.63496023	5.93306182
O	31.17858420	6.31493777	6.75121682
O	31.22538620	8.28448477	8.78426482
H	33.50514120	5.50182777	5.95891082
N	36.05435020	6.41114077	6.94754482
N	36.08860920	7.91351377	8.49882782
N	36.84479320	7.11433577	7.68903082
O	22.17553220	-0.24102223	8.78064382
O	24.13939120	-0.30356223	6.74451182
H	21.33243920	-2.56112423	9.56257882
N	22.20651420	-5.11695523	8.55777882
N	23.70559620	-5.16191123	7.00363582

N	22.89814820	-5.91238923	7.81053882
C	23.40561820	8.51428877	16.74640282
C	22.39327820	7.51743177	16.73140282
C	23.81495320	9.12767177	17.91748182
C	21.76480520	7.10894577	17.88993282
C	23.17301920	8.70847177	19.09004882
C	22.16726520	7.72004677	19.08875782
H	20.99465520	6.34719777	17.85927582
O	22.00598820	6.92389077	15.54740982
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H	24.59071120	9.88404777	17.88742682
N	23.27107120	9.04227377	20.40836882
N	21.73286820	7.52638077	20.38314882
N	22.39365720	8.31623077	21.16327782
H	25.03116920	9.51080977	13.30149382
O	22.46474620	8.73128077	0.04981282
O	24.35678920	6.62800377	-0.00556018
H	21.72427720	9.60143677	-2.27378518
N	24.08717620	7.02498277	-4.86650718
N	23.33280820	7.87893677	-5.62005318
N	22.64293720	8.63035277	-4.82696218
O	15.64002120	6.81605777	8.81756482
H	13.44691520	9.73994177	6.06910482
O	15.72098120	8.84442177	6.84677982
N	10.84445720	8.76958877	7.11448582
N	10.77971020	7.22154177	8.61915982
N	10.03707320	7.99508977	7.89832182
C	22.96061720	16.49159877	7.80107982
C	23.95058520	16.44297277	8.81920682
C	22.42786920	17.68868377	7.36840582
C	24.43228320	17.58762577	9.43004982
C	22.90484920	18.86139477	7.97656582
C	23.88738820	18.79956777	8.98614382
H	25.18775320	17.50898777	10.20328282
O	22.49973820	15.33308777	7.21023282
O	24.47282220	15.24233277	9.23860982
H	21.67355720	17.70631877	6.59057482
N	22.57097320	20.18195877	7.76157882
N	23.27106420	20.92007677	8.55801482
N	24.07535720	20.11072877	9.30959282
H	23.87000620	9.71348577	20.86616682
H	10.42132520	9.43565977	6.48497182
H	24.31720920	-5.63112323	6.35194882
H	36.55396520	8.53192577	9.14689282
H	24.69238620	20.53057677	9.98918182
H	24.69017120	6.36378277	-5.33359018
C	26.85117300	10.26350000	11.47040900
H	27.18431800	10.71565900	12.38116000
C	28.16815100	9.46518500	11.55768300
H	28.48434538	9.19002700	10.57319878
H	28.01209742	8.58245861	12.14192730

H	26.01928500	10.91933700	11.62120700
C	26.53800520	10.45211677	8.50910482
H	27.24299020	9.97836777	7.85836882
C	27.05152020	11.11339777	9.66664882
H	28.08718720	10.90863777	9.84090982
H	26.57338720	11.91991777	10.18221982
H	25.95010320	11.12021577	7.91503782
H	28.92156101	10.06930059	12.01846246

Ni-CFA-1

Zn	-0.89764422	3.05104688	-2.91730132
Cl	-1.20120522	4.64564388	-4.39533232
Zn	-0.22980500	0.28439700	-0.39340200
N	0.98313878	2.51881988	-2.36369432
C	2.19990178	2.95233588	-2.78938532
N	1.19639278	1.57032188	-1.45534832
C	2.55533178	3.93770288	-3.73431132
C	3.90686178	4.13382988	-3.94073532
H	1.78297678	4.51645388	-4.26216232
Zn	-2.00220622	1.30193988	2.56456768
Cl	-2.98970522	1.82892288	4.45803068
N	-2.13600022	2.55776188	0.97939968
C	-2.71606222	3.78748088	0.84506768
N	-1.54472222	2.25403088	-0.17091332
C	-3.48116022	4.55929588	1.73870468
C	-3.96115322	5.78217988	1.27556068
H	-3.70316222	4.18013688	2.74703368
Ni	3.18834394	0.08339414	0.12452824
N	1.95961678	0.68196288	1.58195468
C	2.14865678	0.56208988	2.94337668
N	0.66805978	0.88577788	1.36823968
C	3.30878778	0.40359188	3.72672268
C	3.19586078	0.59641688	5.10071868
N	-1.70866822	3.22602288	-1.06065432
C	-2.44357122	4.21447888	-0.47417332
C	-2.92295622	5.45146888	-0.95318832
C	-3.66701622	6.20646488	-0.06661232
H	-2.69989622	5.78677388	-1.97663632
N	2.49003278	1.36197188	-1.26159032
C	3.17736578	2.20852888	-2.08890432
C	4.55115178	2.40665588	-2.32709732
C	4.91691178	3.38166788	-3.25044032
H	5.32101178	1.80726888	-1.83820632
N	0.00840378	1.03594988	2.51924868
C	0.90824078	0.89680388	3.53421868
C	0.78080878	1.10158688	4.92406368
C	1.92860778	0.94882688	5.67684668
H	-0.18809422	1.38021588	5.36440668
N	-2.55583322	-0.41148212	1.61078068
C	-3.55607922	-1.31306112	1.85346868
N	-1.93896422	-0.76981112	0.48694968

C	-4.48066622	-1.44313412	2.91047168
C	-5.33352122	-2.52875012	2.84905468
H	-4.49666822	-0.72057312	3.73950568
Zn	-1.82022822	-2.64371912	-1.78579332
Cl	-2.78053722	-4.48068912	-2.52592932
N	-1.93922122	-0.93862012	-2.88615732
C	-2.45832422	-0.70879112	-4.12764332
N	-1.44691822	0.20714088	-2.42939132
C	-3.11360422	-1.56035912	-5.03554632
C	-3.57194222	-0.99462612	-6.22302032
N	-2.48961622	-1.86749412	-0.02354032
C	-3.51271822	-2.25398812	0.80002868
C	-4.38813322	-3.35416812	0.74306768
C	-5.30956622	-3.48898012	1.77912268
H	-4.34369622	-4.05374212	-0.10462232
N	-1.61526422	1.18516988	-3.31146532
C	-2.25326422	0.66313688	-4.39745732
C	-2.71149222	1.24614688	-5.59739332
C	-3.36147522	0.40436188	-6.48023732
H	-2.56347122	2.31739888	-5.79785932
N	0.16546278	-2.54927112	-1.46029432
C	1.14599378	-3.50322512	-1.43965332
N	0.75222478	-1.37375112	-1.21191632
C	1.13015478	-4.84688412	-1.86812232
C	2.33947578	-5.51467812	-1.84471532
H	0.19754878	-5.32230512	-2.20653032
N	2.05669478	-1.51654312	-1.04333332
C	2.34019578	-2.88304012	-1.00805832
C	3.56657078	-3.57395612	-0.99056632
C	3.56553078	-4.90095412	-1.41496732
H	4.50415378	-3.06179312	-0.73453332
H	-3.23243722	-2.62952212	-4.80636132
H	4.31974078	0.45154988	3.31512768
C	-4.78060422	6.65200588	2.16235868
C	-4.48682522	6.71836888	3.55916968
C	-5.84374722	7.39764188	1.64744268
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H	-3.63248722	6.14014088	3.94130268
C	-6.59384722	8.18884688	2.53064668
H	-6.11964922	7.35813688	0.58435568
C	-6.28269422	8.23302588	3.90765568
H	-4.95899122	7.52984688	5.51500068
H	-7.36987022	9.41188188	5.36676668
C	6.35653178	3.65544588	-3.50797832
C	6.80997978	3.92472388	-4.83479832
C	7.27374278	3.64528688	-2.45390732
C	8.14001078	4.17887988	-5.13929332
H	6.07416178	3.90603088	-5.65262932
C	8.62260178	3.90095588	-2.74270932
H	6.95690778	3.46966288	-1.41600532
C	9.04418378	4.16408988	-4.06537832

H	8.45960278	4.37247288	-6.17321032
H	11.09562178	4.58040288	-4.63148732
C	4.38721678	0.42773188	5.97635668
C	4.61615778	1.33510088	7.05478168
C	5.71436378	1.24090288	7.89822068
H	3.90280678	2.15915788	7.20534268
C	5.29329378	-0.60950812	5.74465868
C	6.61163178	0.19072288	7.64693968
H	5.86896578	1.96296988	8.71259468
C	6.40868778	-0.72201212	6.58788568
H	5.13412778	-1.34441312	4.94241268
C	-6.27353922	-4.62249712	1.77985768
C	-5.85686622	-5.90742012	1.31404868
C	-6.71288022	-6.99618412	1.27731068
H	-4.81249322	-6.03204812	0.99258768
C	-7.58694822	-4.43011912	2.22269568
C	-8.03337822	-6.80402812	1.71903968
H	-6.38157722	-7.98296412	0.92468668
C	-8.44789522	-5.53520312	2.18237168
H	-7.93211122	-3.44154212	2.55759868
H	10.45299522	-5.09110612	2.88120868
C	-4.28335522	-1.83549312	-7.22349232
C	-4.07098122	-1.62168212	-8.61985932
C	-4.69741722	-2.38630012	-9.59131632
H	-3.36295222	-0.83817512	-8.92726832
C	-5.15135322	-2.84546812	-6.79350532
C	-5.56940422	-3.40099512	-9.16115932
H	-4.52054822	-2.22191712	-10.66351832
C	-5.77997722	-3.61579312	-7.78041832
H	-5.34189222	-3.00802912	-5.72308832
H	-7.09284322	-5.14091412	-6.97228032
C	4.82929778	-5.68640212	-1.43082532
C	5.77208578	-5.53661812	-0.36830432
C	6.97104878	-6.23091212	-0.33700232
H	5.51572578	-4.86389912	0.46370168
C	5.09754678	-6.56267112	-2.48818232
C	7.24439678	-7.10779612	-1.40071532
H	7.68678578	-6.11770012	0.48933968
C	6.31168878	-7.26157712	-2.45119732
H	4.39370278	-6.66894712	-3.32595432
H	6.60512578	-8.56982612	-4.15637232
N	8.33582978	-7.92095912	-1.65076832
N	8.13625378	-8.54828112	-2.76710032
N	6.92519378	-8.16964612	-3.27368232
N	-6.67150522	-4.65626712	-7.76572732
N	-6.98021522	-5.05370012	-9.03515832
N	-6.32966522	-4.31059612	-9.87508432
N	10.77173478	4.23307688	-2.61893932
N	9.72555678	3.96025088	-1.90551432
N	10.39181078	4.36231588	-3.92528532
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N	-8.05247522	9.54065588	3.41872768
N	-7.22360722	9.09201188	4.40868368
N	-9.10297422	-7.67857312	1.79681268
N	10.12722022	-7.03782712	2.26643068
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N	7.44364178	-1.64317212	6.59078268
N	8.25084678	-1.35377412	7.56158368
N	7.77460478	-0.25329412	8.21669868
H	8.29161678	0.11524988	9.01593368
H	-6.05007422	-2.68731112	3.66852768
H	4.23023778	4.91287588	-4.64721932
H	2.37259278	-6.57045812	-2.15178132
H	1.87277778	1.08185188	6.76764468
H	-3.76074522	0.82296688	-7.41576332
H	-4.03906022	7.18991988	-0.38957732
C	5.14813096	0.35715401	0.65890216
H	5.79668696	-0.24610399	1.32461816
H	5.58135496	0.19344001	-0.35284084
C	4.77983496	1.76110871	1.11114160
H	4.34210570	1.77991378	2.13119597
H	5.73246601	2.33699731	1.16547609
H	4.08693782	2.33355574	0.46129029
C	4.29559412	-1.24806009	1.68772089
H	4.42913819	-0.47619785	2.42416824
H	5.23856711	-1.71303602	1.34365002
C	3.08121073	-1.80499344	1.18481772
H	3.18018042	-2.85145910	0.94046366
H	2.12200163	-1.66555674	1.70065347

P1

Ni-MFU-4l

Zn	21.35364700	9.70190800	5.90885500
Cl	20.19472400	11.06566400	4.63568800
Zn	23.26294800	7.49254000	7.98849600
N	22.67335400	10.45563900	7.25676900
C	23.05577400	11.74146800	7.49299800
N	23.37047800	9.66314000	8.07086600
C	22.64171900	12.95517800	6.90680400
C	23.25058300	14.10130000	7.37600300
H	21.87754600	12.99627500	6.11767000
Zn	21.02553300	5.44403300	9.91866200
Cl	19.68158300	4.19453000	11.12115900
N	20.25562000	6.81373300	8.62734300
C	18.97150700	7.16066900	8.32301300
N	21.07137200	7.57334300	7.90037300
C	17.73334100	6.67949300	8.79498600
C	16.60430000	7.26758400	8.25878800
H	17.65670300	5.88162400	9.54673500
Ni	25.36949500	9.45827600	10.19138700
N	23.98332600	8.14270200	10.89597800
C	23.67913400	7.84955800	12.19798000

N	23.17781100	7.42212800	10.12700200
C	24.20938500	8.30828500	13.42156900
C	23.65417900	7.78607100	14.57255300
N	20.37888800	8.40677700	7.12954600
C	19.05208000	8.18856200	7.35511700
C	17.89840700	8.78707500	6.80914100
C	16.68849700	8.31260500	7.27375000
H	17.94737200	9.58611400	6.05630000
N	24.19635500	10.36918400	8.83819300
C	24.03733900	11.68776200	8.51097900
C	24.65823200	12.86537300	8.97869800
C	24.25279600	14.05203700	8.40340900
H	25.43368000	12.86330400	9.75314600
N	22.35512100	6.66798100	10.85236300
C	22.63065900	6.90061800	12.16563800
C	22.06434300	6.36818400	13.34158200
C	22.58851900	6.82293800	14.53546700
H	21.25058200	5.62970900	13.32135800
N	22.34052700	4.55892600	8.63914000
C	22.58607500	3.24791100	8.35248700
N	23.17278400	5.30187100	7.91460400
C	21.99987700	2.05878800	8.83198600
C	22.50102500	0.87918900	8.31714500
H	21.18950800	2.05735600	9.57432500
Zn	25.32875200	5.40247400	5.94224200
Cl	26.60655500	4.14130200	4.67490100
N	24.10107600	6.75767100	5.05012600
C	23.87326500	7.06746800	3.74170100
N	23.33869700	7.54904700	5.79958400
C	24.41185100	6.54545300	2.54786800
C	23.94854300	7.10591100	1.37490800
N	23.95762400	4.53580300	7.16176500
C	23.62992200	3.23291900	7.39830300
C	24.13929900	2.02751900	6.87403700
C	23.56206900	0.86597500	7.34599900
H	24.94885100	2.00136800	6.13147800
N	22.61561900	8.36715800	5.03926100
C	22.91377900	8.10659000	3.73437800
C	22.44373900	8.67632200	2.53348000
C	22.97245700	8.16271300	1.36552800
H	21.69998300	9.48507600	2.51476500
N	26.17969200	6.67453100	7.28057200
C	27.48925800	6.98218400	7.49691300
N	25.44076900	7.42590500	8.09643700
C	28.66663500	6.48771900	6.89860600
C	29.85507000	7.03074000	7.34232500
H	28.64799100	5.71307700	6.11885700
N	26.20432400	8.21565600	8.84693400
C	27.50783500	7.97714200	8.50321000
C	28.72974900	8.53108800	8.94156100
C	29.88081700	8.04711600	8.35558200

H	28.79398800	9.31475000	9.70306100
H	25.15940600	5.74002500	2.54021400
C	23.05139200	8.20446400	-0.99685000
C	24.01817400	7.15797900	-0.98636000
C	22.60016700	8.75928600	-2.18013200
C	24.55513900	6.64330300	-2.15686000
C	23.13421200	8.24881600	-3.37716700
C	24.09281900	7.21072200	-3.35417800
H	25.29811200	5.83681700	-2.10201900
C	32.21283000	7.10681600	7.21354500
C	32.23813600	8.11812500	8.21761300
C	33.37723700	6.62929300	6.64082800
C	33.42609900	8.67295300	8.67002100
C	34.59117700	7.18141600	7.08813300
C	34.60370600	8.18370200	8.08420600
H	33.39927400	9.44976200	9.44549500
C	14.32959100	8.42608900	7.20175100
C	14.24494900	7.39159100	8.17762200
C	13.19868000	9.01840600	6.66016500
C	13.02546600	6.92658700	8.63380800
C	11.96422100	8.54186300	7.12737900
C	11.86766600	7.51652700	8.09512700
H	12.97877100	6.12862600	9.38617900
C	22.43467000	-1.48335400	8.26582200
C	23.48546600	-1.49521400	7.30378900
C	21.86701500	-2.65546300	8.73010500
C	23.99200000	-2.67730600	6.78482500
C	22.36890500	-3.86404600	8.21420000
C	23.41155300	-3.86317800	7.26026900
H	24.80250100	-2.63966200	6.04515800
O	31.01811500	6.57414700	6.78317000
O	31.07408400	8.58231200	8.77732600
H	33.33938900	5.84995600	5.86870200
N	35.89363400	6.91252100	6.71128300
N	35.93823800	8.44859400	8.23568000
N	36.68939500	7.67109200	7.39909500
O	21.95271400	-0.29258700	8.76278000
O	24.03837800	-0.32246100	6.85292800
H	21.05799500	-2.62784200	9.47153500
N	22.01092100	-5.17232900	8.48056500
N	23.60725200	-5.19632700	7.01885800
N	22.75291600	-5.95913200	7.76488100
C	23.62863100	7.71657200	16.93395500
C	22.57145400	6.76221000	16.89787500
C	24.16365500	8.17500600	18.12840900
C	22.02584000	6.24539900	18.05853300
C	23.60539300	7.64646300	19.30242900
C	22.55653500	6.69961800	19.27930500
H	21.21153100	5.51068700	18.01272300
O	22.06060200	6.32548800	15.69600300
O	24.16008400	8.22116300	15.77225400

H	24.97811300	8.91104300	18.10975300
N	23.83053700	7.82205400	20.64121400
N	22.22415000	6.37245600	20.58056900
N	22.98707900	7.04485500	21.38502800
H	25.02719600	9.03852500	13.48538700
O	22.53634900	8.69486900	0.18269500
O	24.45550800	6.61759800	0.19713100
H	21.85488800	9.56515600	-2.16972200
N	24.35287900	7.00423200	-4.68218800
N	23.61323100	7.84813200	-5.46252800
N	22.88365200	8.59378300	-4.69204300
O	15.38696300	6.82246500	8.69675200
H	13.31055500	9.81244200	5.91021400
O	15.54851000	8.87662700	6.75966600
N	10.65423800	8.84040700	6.86539600
N	10.53164300	7.26862600	8.34861300
N	9.81602400	8.06099100	7.61243400
C	23.47527500	16.45131700	7.27579500
C	24.47208500	16.40229700	8.29322600
C	23.08229300	17.64892800	6.70723500
C	25.09700100	17.54792400	8.76324000
C	23.70586900	18.82064300	7.17284900
C	24.69328500	18.75966600	8.18190300
H	25.86000300	17.46445600	9.54829900
O	22.87191000	15.29735100	6.82843800
O	24.85102300	15.20593800	8.84909200
H	22.31295100	17.66811700	5.92445800
N	23.52733100	20.14095700	6.80449100
N	24.32659500	20.87992800	7.50931200
N	25.04233400	20.07280200	8.34897700
H	24.50629900	8.42266800	21.11444200
H	10.25969500	9.52801700	6.22277600
H	24.26965400	-5.65352000	6.39149200
H	36.40382700	9.11164100	8.85609100
H	25.72574500	20.48908100	8.98217300
H	24.98960200	6.34094800	-5.12496100
C	26.74756700	10.73575200	10.79351700
H	27.38162700	11.08909800	9.95094500
C	27.59740000	10.10632100	11.91017600
H	27.90880500	9.06718600	11.64674300
H	26.98221200	9.98797900	12.83182300
H	26.21867200	11.63239500	11.19335100
C	28.86664200	10.89235500	12.27502800
H	29.49722500	10.99512300	11.36261000
H	28.57782300	11.93035400	12.55187500
C	29.68248400	10.25205100	13.39857100
H	30.00884000	9.22693900	13.12381700
H	30.59187500	10.84068200	13.63529300
H	29.08680200	10.16794600	14.33173700

Ni-CFA-1

Zn	-0.65060900	2.94491100	-2.69808200
Cl	-0.90946300	4.54965100	-4.17443500
Zn	-0.22959200	0.30139500	-0.30848000
N	1.21051300	2.38073700	-2.11377500
C	2.43472400	2.81918900	-2.52340200
N	1.40876900	1.40923900	-1.21251500
C	2.83273800	3.80218100	-3.45367100
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90783800	1.20907200	2.76744700
Cl	-2.93116600	1.77532700	4.62705300
N	-1.93757000	2.48278700	1.18351800
C	-2.52180400	3.70875200	1.03041100
N	-1.32705100	2.17418700	0.04391200
C	-3.28517600	4.49134500	1.91600000
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.26482600	-0.23207300	0.33145400
N	1.97198400	0.17869200	1.84687800
C	2.24952000	0.36736900	3.19024300
N	0.66642200	0.40994200	1.65484700
C	3.39346000	0.15236400	3.97728000
C	3.27564200	0.32180400	5.35402100
N	-1.48173300	3.14068400	-0.85425900
C	-2.22727800	4.13298200	-0.28494400
C	-2.68118300	5.37805100	-0.76767300
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69277700	1.19392600	-0.99531600
C	3.38407300	2.05257300	-1.80934300
C	4.76566800	2.21598400	-2.01818700
C	5.17329100	3.18510400	-2.93034200
H	5.49198400	1.57920100	-1.49268300
N	0.07379500	0.77749800	2.79043300
C	1.01305700	0.72855400	3.77004600
C	0.88044600	0.91427100	5.16239800
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48728600	-0.45877700	1.75237600
C	-3.45841300	-1.38129000	2.01244000
N	-1.88972400	-0.80078800	0.61586700
C	-4.39762400	-1.50246100	3.05748300
C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.70049600	-2.72728700	-1.60288000
Cl	-2.64733100	-4.55160000	-2.38471300
N	-1.73402600	-1.02968400	-2.72085700
C	-2.26408000	-0.77700400	-3.95372000
N	-1.21565000	0.10257600	-2.25792700
C	-2.92036300	-1.61553000	-4.87284000
C	-3.35131100	-1.04003100	-6.06579400

N	-2.42156000	-1.90893400	0.11381100
C	-3.41786500	-2.31659000	0.95387600
C	-4.31060000	-3.40170300	0.87962800
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37561400	1.09162900	-3.12979300
C	-2.03120800	0.59171800	-4.21779600
C	-2.46163500	1.18452300	-5.42315900
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27211600	-2.70121700	-1.14003400
C	1.26076200	-3.63215500	-1.23685800
N	0.82042000	-1.57882500	-0.67018100
C	1.24385100	-4.97590400	-1.66654200
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12186100	-1.72952100	-0.45918900
C	2.45776400	-3.02007900	-0.80025200
C	3.68414000	-3.70930700	-0.78604900
C	3.67973700	-5.03713400	-1.20458400
H	4.61466600	-3.21412200	-0.48496900
H	-3.05604700	-2.68397400	-4.64962800
H	4.19925300	-0.53509700	3.73826200
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700
C	6.44294800	-1.15739500	6.77383300

H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400
H	-5.99866300	-2.72322600	3.78737900

H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	5.04316000	0.23595900	1.06328200
H	5.70159200	0.70628700	0.30173300
H	4.93671600	0.96899900	1.89107500
C	5.65417800	-1.08459900	1.55136500
H	5.94581900	-1.71303400	0.67797300
C	6.88338500	-0.94059700	2.47141500
H	7.66310700	-0.35742600	1.93449400
H	6.60037800	-0.31792500	3.34948500
C	7.44817900	-2.28116700	2.94160300
H	6.67993600	-2.87997100	3.47583800
H	7.80576100	-2.89192700	2.08541800
H	4.89940200	-1.70186900	2.10131200
H	8.29261300	-2.15260200	3.64724400

I2

Ni-MFU-4l

Zn	21.49659000	9.71176400	5.82173800
Cl	20.27275100	11.04836200	4.60587700
Zn	23.46934300	7.53486600	7.84001200
N	22.81200400	10.49211200	7.13505400
C	23.07253000	11.77620000	7.49300100
N	23.59238000	9.70048000	7.86582400
C	22.52663000	12.99033300	7.03650800
C	23.01084300	14.13590900	7.62817500
H	21.76619700	13.03128300	6.26410000
Zn	21.34780500	5.53912600	9.87588800
Cl	20.03453200	4.33704300	11.14152300
N	20.49340600	6.86342100	8.59773200
C	19.20161200	7.19011300	8.32462500
N	21.27681100	7.62015100	7.83824600
C	17.98644700	6.70300400	8.84091100
C	16.83926300	7.27126000	8.33041500
H	17.94345100	5.92689100	9.59725200
Ni	25.78531903	9.61175649	9.88251123
N	24.29420100	8.29840100	10.74536700
C	23.87055200	8.13747600	12.04422100
N	23.52403800	7.50138900	9.99798400
C	24.27437800	8.74407500	13.25008600
C	23.63916300	8.32347300	14.39703300
N	20.55536200	8.43166900	7.07461100
C	19.24204500	8.20160600	7.34217700
C	18.06896800	8.78018600	6.82300700
C	16.88243300	8.29986500	7.33101100
H	18.08779400	9.55917100	6.06864500
N	24.34070700	10.40286700	8.70483500
C	24.06458400	11.72296300	8.49591700

C	24.54812200	12.90049300	9.09924400
C	24.01114000	14.08688000	8.65212600
H	25.29371800	12.89428300	9.88244300
N	22.67016300	6.80035200	10.73775600
C	22.85034900	7.16164900	12.03435600
C	22.20411200	6.73082800	13.20796300
C	22.61512500	7.32257600	14.38153100
H	21.42348400	5.97773600	13.19771100
N	22.57372500	4.59852800	8.56428100
C	22.79555800	3.28686600	8.27974700
N	23.35827500	5.32635200	7.77993400
C	22.23669600	2.10936500	8.81008200
C	22.70120900	0.92487000	8.28017000
H	21.48333100	2.12140900	9.59020900
Zn	25.39481700	5.39819100	5.69733600
Cl	26.61146200	4.11859300	4.41163400
N	24.16174300	6.75880300	4.84267200
C	23.89665200	7.07739700	3.54695400
N	23.43421400	7.55480300	5.61657100
C	24.38842100	6.55259400	2.33748200
C	23.89435300	7.12328500	1.18537800
N	24.09043600	4.55029500	6.98931200
C	23.77402600	3.25606000	7.26406900
C	24.24650400	2.04503400	6.72534100
C	23.69672800	0.89528400	7.24786500
H	24.99904500	2.00776600	5.94522600
N	22.70078600	8.38547100	4.88562400
C	22.95414100	8.12646200	3.57418400
C	22.45219600	8.70608100	2.39435000
C	22.93538200	8.18966400	1.21132800
H	21.72690200	9.51238000	2.40373200
N	26.33945600	6.63762200	6.99712400
C	27.64699500	6.88201000	7.27556200
N	25.60661800	7.41303100	7.78742500
C	28.82836900	6.34136200	6.73588500
C	30.01136300	6.82371800	7.25260700
H	28.81903300	5.58754000	5.95600500
N	26.37085300	8.18439100	8.56886000
C	27.66443900	7.86192600	8.29104800
C	28.87767100	8.35051900	8.81184300
C	30.03333700	7.82029000	8.28185200
H	28.92418300	9.10349600	9.58999500
H	25.11400300	5.74719800	2.30342000
C	22.93429100	8.23582600	-1.15366000
C	23.88411800	7.17991300	-1.17815200
C	22.44919900	8.79853100	-2.31631300
C	24.37359600	6.65923400	-2.36309300
C	22.93420700	8.28321100	-3.52957100
C	23.87717700	7.23470900	-3.54004100
H	25.09793000	5.85330800	-2.33941900
C	32.37570200	6.78343400	7.25220500

C	32.39677300	7.77170000	8.27233300
C	33.54062900	6.25739000	6.73248800
C	33.57973900	8.25923300	8.79917000
C	34.75185100	6.73998500	7.25438800
C	34.75891600	7.72117400	8.26722300
H	33.55377300	9.01338500	9.57722900
C	14.52001200	8.39130000	7.33219700
C	14.47598100	7.37323100	8.32164400
C	13.37144700	8.96757000	6.81900700
C	13.27935900	6.90485300	8.82400800
C	12.15966400	8.48772200	7.33290200
C	12.10209000	7.47761400	8.31531000
H	13.26508500	6.12745400	9.57882700
C	22.62520600	-1.43928500	8.26392700
C	23.61119400	-1.46741200	7.24182900
C	22.08444900	-2.59974300	8.77841100
C	24.08224200	-2.65378200	6.70760000
C	22.55007100	-3.81441700	8.24873100
C	23.52936200	-3.82846800	7.23410200
H	24.83550100	-2.63284000	5.92856200
O	31.17908400	6.31705800	6.74671700
O	31.22588600	8.28660500	8.77976500
H	33.50564100	5.50394800	5.95441100
N	36.05485000	6.41326100	6.94304500
N	36.08910900	7.91563400	8.49432800
N	36.84529300	7.11645600	7.68453100
O	22.17603200	-0.23890200	8.77614400
O	24.13989100	-0.30144200	6.74001200
H	21.33293900	-2.55900400	9.55807900
N	22.20701400	-5.11483500	8.55327900
N	23.70609600	-5.15979100	6.99913600
N	22.89864800	-5.91026900	7.80603900
C	23.40611800	8.51640900	16.74190300
C	22.39377800	7.51955200	16.72690300
C	23.81545300	9.12979200	17.91298200
C	21.76530500	7.11106600	17.88543300
C	23.17351900	8.71059200	19.08554900
C	22.16776500	7.72216700	19.08425800
H	20.99515500	6.34931800	17.85477600
O	22.00648800	6.92601100	15.54291000
O	24.02417400	8.91184800	15.57891800
H	24.59121100	9.88616800	17.88292700
N	23.27157100	9.04439400	20.40386900
N	21.73336800	7.52850100	20.37864900
N	22.39415700	8.31835100	21.15877800
H	25.03166000	9.51293900	13.29699300
O	22.46524600	8.73340100	0.04531300
O	24.35728900	6.63012400	-0.01006000
H	21.72477700	9.60355700	-2.27828500
N	24.08767600	7.02710300	-4.87100700
N	23.33330800	7.88105700	-5.62455300

N	22.64343700	8.63247300	-4.83146200
O	15.64052100	6.81817800	8.81306500
H	13.44741500	9.74206200	6.06460500
O	15.72148100	8.84654200	6.84228000
N	10.84495700	8.77170900	7.10998600
N	10.78021000	7.22366200	8.61466000
N	10.03757300	7.99721000	7.89382200
C	22.96111700	16.49371900	7.79658000
C	23.95108500	16.44509300	8.81470700
C	22.42836900	17.69080400	7.36390600
C	24.43278300	17.58974600	9.42555000
C	22.90534900	18.86351500	7.97206600
C	23.88788800	18.80168800	8.98164400
H	25.18825300	17.51110800	10.19878300
O	22.50023800	15.33520800	7.20573300
O	24.47332200	15.24445300	9.23411000
H	21.67405700	17.70843900	6.58607500
N	22.57147300	20.18407900	7.75707900
N	23.27156400	20.92219700	8.55351500
N	24.07585700	20.11284900	9.30509300
H	23.87050600	9.71560600	20.86166700
H	10.42182500	9.43778000	6.48047200
H	24.31770900	-5.62900300	6.34744900
H	36.55446500	8.53404600	9.14239300
H	24.69288600	20.53269700	9.98468200
H	24.69067100	6.36590300	-5.33809000
C	25.58111603	10.70211049	11.51943523
H	25.50877403	11.79214449	11.37692323
C	26.60836103	10.39879049	12.61420923
H	27.43630103	11.13770649	12.56820523
H	26.12526603	10.61002849	13.60049723
C	26.94428303	10.76103549	8.65552823
H	27.38900403	10.07384949	7.92195123
C	27.51574203	10.94988849	9.91395723
H	27.31072503	11.88408749	10.45182823
H	28.43608003	10.45398849	10.24568323
H	26.30438403	11.54551149	8.22743723
H	24.55777603	10.34451849	11.73421723
C	27.22980503	8.98797849	12.66607123
H	26.47135903	8.21783749	12.41694223
H	27.99373303	8.90010249	11.86606823
C	27.85815003	8.67093449	14.02329623
H	28.35249303	7.67914249	14.02297523
H	28.62116103	9.42704149	14.30458723
H	27.08933903	8.66167149	14.82454623

Ni-CFA-1

Zn	-0.76455000	2.89294100	-2.75684900
Cl	-1.06482200	4.48917200	-4.23566000
Zn	-0.22066500	0.27137600	-0.38161300
N	1.11948300	2.36244300	-2.20391200

C	2.33627300	2.79586100	-2.62971200
N	1.33297000	1.41424200	-1.29529900
C	2.69171000	3.78122500	-3.57464700
C	4.04324000	3.97736600	-3.78105600
H	1.91935500	4.35999000	-4.10248300
Zn	-1.86334600	1.14604800	2.72481500
Cl	-2.85332200	1.67248200	4.61770600
N	-1.99962900	2.40127500	1.13907000
C	-2.57968700	3.63101600	1.00474500
N	-1.40834200	2.09756500	-0.01118800
C	-3.34478000	4.40283300	1.89838500
C	-3.82477500	5.62571600	1.43524000
H	-3.56678400	4.02367300	2.90671300
Ni	3.27955695	-0.10845247	0.20083316
N	2.07189200	0.39123000	1.74327200
C	2.28484400	0.40570600	3.10294500
N	0.80427600	0.72905300	1.52792800
C	3.44519900	0.24727300	3.88638300
C	3.33225200	0.44001000	5.26039100
N	-1.57230200	3.06957300	-0.90097100
C	-2.30719800	4.05801200	-0.31449500
C	-2.78657800	5.29500500	-0.79350900
C	-3.53063800	6.05000100	0.09306700
H	-2.56351800	5.63031000	-1.81695700
N	2.62873800	1.19766500	-1.10985600
C	3.31396100	2.05199200	-1.92954600
C	4.68752300	2.25012500	-2.16751200
C	5.05328900	3.22517100	-3.09079600
H	5.45739100	1.65083200	-1.67849600
N	0.14473000	0.87930800	2.67891800
C	1.04460900	0.74024100	3.69390900
C	0.91720100	0.94518000	5.08373600
C	2.06498600	0.79236300	5.83652600
H	-0.05171600	1.22375200	5.52408600
N	-2.41947300	-0.56797100	1.77047600
C	-3.41970400	-1.46952200	2.01314700
N	-1.80258500	-0.92630200	0.64667100
C	-4.34428800	-1.59959800	3.07015100
C	-5.19714300	-2.68521400	3.00873400
H	-4.36029000	-0.87703700	3.89918500
Zn	-1.68716900	-2.79828200	-1.62981400
Cl	-2.64414900	-4.63715400	-2.36625000
N	-1.80283400	-1.09508800	-2.72647600
C	-2.32193800	-0.86525800	-3.96796800
N	-1.31053700	0.05066500	-2.26966800
C	-2.97722600	-1.71682300	-4.87586700
C	-3.43556400	-1.15109000	-6.06334100
N	-2.35325000	-2.02395500	0.13614000
C	-3.37634300	-2.41045000	0.95970500
C	-4.25175500	-3.51063200	0.90274700
C	-5.17318800	-3.64544400	1.93880200

H	-4.20731800	-4.21020600	0.05505700
N	-1.47890400	1.02872000	-3.15176000
C	-2.11688500	0.50667400	-4.23777900
C	-2.57511200	1.08968300	-5.43771500
C	-3.22509700	0.24789800	-6.32055800
H	-2.42709300	2.16093500	-5.63818000
N	0.30170100	-2.70565500	-1.30063300
C	1.28240900	-3.65975300	-1.27999700
N	0.88891000	-1.53039700	-1.05234000
C	1.26653900	-5.00334000	-1.70846800
C	2.47585400	-5.67114200	-1.68503600
H	0.33392700	-5.47876900	-2.04685100
N	2.17396800	-1.68712400	-0.70130500
C	2.47637600	-3.03937800	-0.84818800
C	3.70295700	-3.73040800	-0.83095800
C	3.70191300	-5.05741100	-1.25531000
H	4.64052800	-3.21826300	-0.57482700
H	-3.09605900	-2.78598600	-4.64668200
H	4.45611800	0.29505200	3.47480100
C	-4.64422600	6.49554200	2.32203800
C	-4.35044700	6.56190500	3.71884900
C	-5.70736900	7.24117800	1.80712200
C	-5.08036500	7.33865400	4.60658400
H	-3.49610900	5.98367700	4.10098200
C	-6.45746900	8.03238300	2.69032600
H	-5.98327100	7.20167300	0.74403500
C	-6.14631600	8.07656200	4.06733500
H	-4.82261300	7.37338300	5.67468000
H	-7.23349200	9.25541800	5.52644600
C	6.49291000	3.49898200	-3.34829900
C	6.94635800	3.76826000	-4.67511900
C	7.41012100	3.48882300	-2.29422800
C	8.27638900	4.02241600	-4.97961400
H	6.21054000	3.74956700	-5.49295000
C	8.75898000	3.74449200	-2.58303000
H	7.09328600	3.31319900	-1.25632600
C	9.18056200	4.00762600	-3.90569900
H	8.59598100	4.21600900	-6.01353100
H	11.23200000	4.42393900	-4.47180800
C	4.52359500	0.27126800	6.13603600
C	4.75253600	1.17863700	7.21446100
C	5.85074200	1.08443900	8.05790000
H	4.03918500	2.00269400	7.36502200
C	5.42967200	-0.76597200	5.90433800
C	6.74801000	0.03425900	7.80661900
H	6.00534400	1.80650600	8.87227400
C	6.54506600	-0.87847600	6.74756500
H	5.27050600	-1.50087700	5.10209200
C	-6.13716100	-4.77896100	1.93953700
C	-5.72048800	-6.06388400	1.47372800
C	-6.57650200	-7.15264800	1.43699000

H	-4.67611500	-6.18851200	1.15226700
C	-7.45057000	-4.58658300	2.38237500
C	-7.89700000	-6.96049200	1.87871900
H	-6.24519900	-8.13942800	1.08436600
C	-8.31151700	-5.69166700	2.34205100
H	-7.79573300	-3.59800600	2.71727800
H	-10.31661700	-5.24757000	3.04088800
C	-4.14697700	-1.99195700	-7.06381300
C	-3.93460300	-1.77814600	-8.46018000
C	-4.56103900	-2.54276400	-9.43163700
H	-3.22657400	-0.99463900	-8.76758900
C	-5.01497500	-3.00193200	-6.63382600
C	-5.43302600	-3.55745900	-9.00148000
H	-4.38417000	-2.37838100	-10.50383900
C	-5.64359900	-3.77225700	-7.62073900
H	-5.20551400	-3.16449300	-5.56340900
H	-6.95646500	-5.29737800	-6.81260100
C	4.96567600	-5.84286600	-1.27114600
C	5.90846400	-5.69308200	-0.20862500
C	7.10742700	-6.38737600	-0.17732300
H	5.65210400	-5.02036300	0.62338100
C	5.23392500	-6.71913500	-2.32850300
C	7.38077500	-7.26426000	-1.24103600
H	7.82316400	-6.27416400	0.64901900
C	6.44806700	-7.41804100	-2.29151800
H	4.53008100	-6.82541100	-3.16627500
H	6.74150400	-8.72629000	-3.99669300
N	8.47220800	-8.07742300	-1.49108900
N	8.27263200	-8.70474500	-2.60742100
N	7.06157200	-8.32611000	-3.11400300
N	-6.53512700	-4.81273100	-7.60604800
N	-6.84383700	-5.21016400	-8.87547900
N	-6.19328700	-4.46706000	-9.71540500
N	10.90811300	4.07661300	-2.45926000
N	9.86193500	3.80378700	-1.74583500
N	10.52818900	4.20585200	-3.76560600
N	-7.55074100	8.85122200	2.45580900
N	-7.91609700	9.38419200	3.57840700
N	-7.08722900	8.93554800	4.56836300
N	-8.96659600	-7.83503700	1.95649200
N	-9.99084200	-7.19429100	2.42611000
N	-9.62671200	-5.89969900	2.66618300
N	7.58002000	-1.79963600	6.75046200
N	8.38722500	-1.51023800	7.72126300
N	7.91098300	-0.40975800	8.37637800
H	8.42799500	-0.04121400	9.17561300
H	-5.91369600	-2.84377500	3.82820700
H	4.36661600	4.75641200	-4.48754000
H	2.50897100	-6.72692200	-1.99210200
H	2.00915600	0.92538800	6.92732400
H	-3.62436700	0.66650300	-7.25608400

H	-3.90268200	7.03345600	-0.22989800
C	4.27323995	1.47104653	0.90158516
H	4.82327495	1.11178353	1.79003116
H	5.00985295	1.67066253	0.10621016
C	3.45958695	2.71606953	1.20503116
H	2.91201295	2.60682153	2.16370516
H	2.68638195	2.89638053	0.43038016
C	4.97878995	-0.91779147	-0.41575184
H	5.81384495	-0.21032447	-0.54233284
H	4.75784195	-1.51639447	-1.31308884
C	4.64362895	-1.35227347	0.89689816
H	4.13907595	-2.31359747	1.08630116
H	5.22935095	-0.98040747	1.75132716
C	4.36022495	3.96359653	1.28289316
H	5.15400795	3.80035453	2.04489816
H	4.88912895	4.08810753	0.31194216
C	3.57472395	5.23407353	1.61073716
H	2.79756095	5.43226353	0.84338216
H	3.05864395	5.14784253	2.58958416
H	4.23683495	6.12190353	1.65626716

TS-I2

Ni-MFU-4l

Zn	21.47120200	9.72095400	5.79702300
Cl	20.23479600	11.05906400	4.57114200
Zn	23.47702000	7.53187100	7.83993600
N	22.78327900	10.49582400	7.13009200
C	23.07256800	11.77618900	7.49296500
N	23.51535200	9.69549300	7.90300600
C	22.52664100	12.99033400	7.03649700
C	23.01084300	14.13590900	7.62817500
H	21.75549300	13.03313600	6.25441700
Zn	21.32385500	5.51106000	9.87888100
Cl	20.01420600	4.31984600	11.17636900
N	20.49919200	6.86249700	8.59766600
C	19.20161200	7.19011700	8.32462800
N	21.28919900	7.61868200	7.83813100
C	17.98644700	6.70300300	8.84091000
C	16.83926300	7.27126000	8.33041500
H	17.94149800	5.91706900	9.60766900
Ni	25.56779843	9.59167450	9.94840122
N	24.26000200	8.29736000	10.73960300
C	23.87035700	8.13767000	12.04441600
N	23.51814300	7.45260700	10.00385100
C	24.27437700	8.74408800	13.25008000
C	23.63918800	8.32344800	14.39703700
N	20.56131200	8.42891500	7.07447800
C	19.24204500	8.20160900	7.34218100
C	18.06896800	8.78018500	6.82300600
C	16.88243300	8.29986500	7.33101100

H	18.08769200	9.56918400	6.05815400
N	24.29312200	10.39700200	8.72251300
C	24.06423800	11.72298600	8.49631500
C	24.54810600	12.90049300	9.09925800
C	24.01117600	14.08688300	8.65209100
H	25.28607500	12.90089400	9.90621000
N	22.66330100	6.76761800	10.74774800
C	22.85038400	7.16161700	12.03430700
C	22.20412600	6.73081300	13.20796500
C	22.61512500	7.32257600	14.38153100
H	21.41384900	5.96649900	13.19611700
N	22.58052900	4.60402900	8.57097500
C	22.79555300	3.28686600	8.27974300
N	23.37144800	5.33970600	7.79382700
C	22.23669700	2.10936500	8.81008300
C	22.70120900	0.92487000	8.28017000
H	21.47376600	2.11970600	9.60097400
Zn	25.41316600	5.40274000	5.69839300
Cl	26.65753100	4.12118000	4.42207400
N	24.16173600	6.76262300	4.84986900
C	23.89664700	7.07739300	3.54695400
N	23.43801600	7.56272000	5.63012200
C	24.38842200	6.55259500	2.33748200
C	23.89435300	7.12328500	1.18537800
N	24.09662700	4.55741200	6.99874600
C	23.77402700	3.25606000	7.26406800
C	24.24650300	2.04503400	6.72534000
C	23.69672800	0.89528400	7.24786500
H	25.01043500	2.00631600	5.93638800
N	22.70384200	8.38971900	4.89043300
C	22.95413500	8.12645800	3.57418400
C	22.45219800	8.70608300	2.39435000
C	22.93538200	8.18966400	1.21132800
H	21.71665300	9.52256100	2.40313500
N	26.32812300	6.65471600	6.99588300
C	27.64698900	6.88197400	7.27559600
N	25.59975300	7.41683200	7.81160600
C	28.82836900	6.34137500	6.73587300
C	30.01136300	6.82371800	7.25260700
H	28.81803200	5.57879400	5.94424400
N	26.36347000	8.14787100	8.61800400
C	27.66454700	7.86172100	8.29093200
C	28.87763000	8.35060500	8.81185900
C	30.03333700	7.82029400	8.28184900
H	28.94795800	9.10404600	9.60584600
H	25.12401600	5.73700300	2.30206800
C	22.93429100	8.23582600	-1.15366000
C	23.88411800	7.17991300	-1.17815200
C	22.44919900	8.79853100	-2.31631300
C	24.37359600	6.65923400	-2.36309300
C	22.93420700	8.28321100	-3.52957100

C	23.87717700	7.23470900	-3.54004100
H	25.10714500	5.84288100	-2.33464100
C	32.37570200	6.78343400	7.25220500
C	32.39677300	7.77170000	8.27233300
C	33.54062900	6.25739000	6.73248800
C	33.57973900	8.25923300	8.79917000
C	34.75185100	6.73998500	7.25438800
C	34.75891600	7.72117400	8.26722300
H	33.54968200	9.02371200	9.58660200
C	14.52001200	8.39130000	7.33219700
C	14.47598100	7.37323100	8.32164400
C	13.37144700	8.96757000	6.81900700
C	13.27935900	6.90485300	8.82400800
C	12.15966400	8.48772200	7.33290200
C	12.10209000	7.47761400	8.31531000
H	13.26429100	6.11736800	9.58859500
C	22.62520600	-1.43928500	8.26392700
C	23.61119400	-1.46741200	7.24182900
C	22.08444900	-2.59974300	8.77841100
C	24.08224200	-2.65378200	6.70760000
C	22.55007100	-3.81441700	8.24873100
C	23.52936200	-3.82846800	7.23410200
H	24.84522600	-2.62807300	5.91859600
O	31.17984300	6.31910500	6.74845100
O	31.22608200	8.28651500	8.77700500
H	33.50580900	5.49430000	5.94415200
N	36.05818600	6.41212000	6.94174300
N	36.09488300	7.91717700	8.49591400
N	36.85133300	7.11794300	7.68583700
O	22.17826600	-0.24031000	8.77453600
O	24.13860400	-0.30239000	6.74213800
H	21.32313800	-2.55910400	9.56817200
N	22.20589200	-5.11832000	8.55457700
N	23.70753900	-5.16562500	6.99750600
N	22.90006000	-5.91654400	7.80460200
C	23.40611800	8.51640900	16.74190300
C	22.39377800	7.51955200	16.72690300
C	23.81545300	9.12979200	17.91298200
C	21.76530500	7.11106600	17.88543300
C	23.17351900	8.71059200	19.08554900
C	22.16776500	7.72216700	19.08425800
H	20.98499100	6.33954100	17.85512100
O	22.00940200	6.92827400	15.54348600
O	24.02417300	8.90772800	15.57782500
H	24.60130200	9.89576300	17.87891800
N	23.27259600	9.04666000	20.40947200
N	21.73186800	7.52760400	20.38203000
N	22.39509700	8.32045400	21.16447400
H	25.04732500	9.52320500	13.29949700
O	22.46734600	8.73157700	0.04372900
O	24.35603400	6.63222000	-0.01098900

H	21.71535500	9.61399200	-2.27832800
N	24.08921400	7.02550100	-4.87684800
N	23.33479200	7.87960700	-5.63086400
N	22.64242300	8.63380300	-4.83498300
O	15.63912500	6.82043300	8.81145000
H	13.45292700	9.75173400	6.05495300
O	15.72031400	8.84501900	6.84415700
N	10.83924300	8.77358700	7.10834500
N	10.77661200	7.22267800	8.61579800
N	10.03137400	7.99905400	7.89227000
C	22.96111700	16.49371900	7.79658000
C	23.95108500	16.44509300	8.81470700
C	22.42836900	17.69080400	7.36390600
C	24.43278300	17.58974600	9.42555000
C	22.90534900	18.86351500	7.97206600
C	23.88788800	18.80168800	8.98164400
H	25.19680100	17.50564700	10.20948200
O	22.49930300	15.33636600	7.20951800
O	24.46898100	15.24524000	9.23610700
H	21.66357600	17.70902500	6.57668800
N	22.57000800	20.18753700	7.75643300
N	23.27233100	20.92840900	8.55607800
N	24.07694100	20.11851200	9.30750500
H	23.88096500	9.72800200	20.86456500
H	10.41974100	9.44937700	6.46900500
H	24.32862100	-5.63196800	6.33556500
H	36.55765800	8.54569400	9.15343500
H	24.70323900	20.53469600	9.99726900
H	24.70128500	6.35370200	-5.34100800
C	27.04879169	10.72631454	9.51200243
H	27.62889769	10.26979554	8.69942443
C	27.21005443	10.34255550	10.88247922
H	27.52542543	9.29317950	11.07831522
H	27.77457743	10.99286150	11.57080022
H	26.85232069	11.79322254	9.32511843
C	25.47195127	10.98477896	11.57522795
H	25.82772027	10.71836296	12.58996495
H	25.89733627	11.98919596	11.37796595
C	23.93840027	11.17438796	11.61700295
H	23.36572727	10.23450096	11.58880795
H	23.59632927	11.74554796	10.73737595
C	23.53880127	11.95510196	12.88149895
H	24.09134427	12.92087796	12.91273095
H	23.85905627	11.39030596	13.78553695
C	22.03234327	12.21168296	12.94524895
H	21.75180627	12.77792896	13.85586495
H	21.68472927	12.79292896	12.06607395
H	21.46647427	11.25698996	12.95517095

Ni-CFA-1

Zn -0.80801800 2.88533200 -2.77770300

Cl	-1.10896400	4.48087100	-4.25783200
Zn	-0.25726700	0.27400300	-0.39452500
N	1.07538000	2.35404700	-2.22619400
C	2.29214300	2.78756300	-2.65188500
N	1.28863400	1.40554900	-1.31784800
C	2.64757300	3.77293000	-3.59681100
C	3.99910300	3.96905700	-3.80323500
H	1.87521800	4.35168100	-4.12466200
Zn	-1.90021700	1.13781300	2.70534100
Cl	-2.89746400	1.66415000	4.59553100
N	-2.04375900	2.39298900	1.11690000
C	-2.62382100	3.62270800	0.98256800
N	-1.45248100	2.08925800	-0.03341300
C	-3.38891900	4.39452300	1.87620500
C	-3.86891200	5.61740700	1.41306100
H	-3.61092100	4.01536400	2.88453400
Ni	3.25973144	-0.35336195	0.25322487
N	2.03256000	0.41433000	1.72105900
C	2.24089800	0.39731700	3.08087700
N	0.76030100	0.72100500	1.50574000
C	3.40102900	0.23881900	3.86422300
C	3.28810200	0.43164400	5.23821900
N	-1.61642700	3.06125000	-0.92315400
C	-2.35133000	4.04970600	-0.33667300
C	-2.83071500	5.28669600	-0.81568800
C	-3.57477500	6.04169200	0.07088800
H	-2.60765500	5.62200100	-1.83913600
N	2.58839600	1.16446200	-1.13155000
C	3.26960700	2.04375600	-1.95140400
C	4.64339300	2.24188300	-2.18959700
C	5.00915300	3.21689500	-3.11294000
H	5.41325300	1.64249600	-1.70070600
N	0.10064500	0.87117700	2.65674900
C	1.00048200	0.73203100	3.67171900
C	0.87305000	0.93681400	5.06156400
C	2.02084900	0.78405400	5.81434700
H	-0.09585300	1.21544300	5.50190700
N	-2.46359200	-0.57625500	1.74828100
C	-3.46383800	-1.47783400	1.99096900
N	-1.84672300	-0.93458400	0.62445000
C	-4.38842500	-1.60790700	3.04797200
C	-5.24128000	-2.69352300	2.98655500
H	-4.40442700	-0.88534600	3.87700600
Zn	-1.73540100	-2.80345900	-1.65216700
Cl	-2.68829600	-4.64546200	-2.38842900
N	-1.84698000	-1.10339300	-2.74865700
C	-2.36608300	-0.87356400	-3.99014300
N	-1.35467700	0.04236800	-2.29189100
C	-3.02136300	-1.72513200	-4.89804600
C	-3.47970100	-1.15939900	-6.08552000
N	-2.39737500	-2.03226700	0.11396000

C	-3.42047700	-2.41876100	0.93752900
C	-4.29589200	-3.51894100	0.88056800
C	-5.21732500	-3.65375300	1.91662300
H	-4.25145500	-4.21851500	0.03287800
N	-1.52302300	1.02039700	-3.17396500
C	-2.16102300	0.49836400	-4.25995700
C	-2.61925100	1.08137400	-5.45989300
C	-3.26923400	0.23958900	-6.34273700
H	-2.47123000	2.15262600	-5.66035900
N	0.25770400	-2.71404400	-1.32279400
C	1.23823500	-3.66799800	-1.30215300
N	0.84446600	-1.53852400	-1.07441600
C	1.22239600	-5.01165700	-1.73062200
C	2.43171700	-5.67945100	-1.70721500
H	0.28979000	-5.48707800	-2.06903000
N	2.13318700	-1.70433800	-0.72470800
C	2.43243700	-3.04781300	-0.87055800
C	3.65881200	-3.73872900	-0.85306600
C	3.65777200	-5.06572700	-1.27746700
H	4.59639500	-3.22656600	-0.59703300
H	-3.14019600	-2.79429500	-4.66886100
H	4.41198200	0.28677700	3.45262800
C	-4.68836300	6.48723300	2.29985900
C	-4.39458400	6.55359600	3.69667000
C	-5.75150600	7.23286900	1.78494300
C	-5.12450200	7.33034500	4.58440500
H	-3.54024600	5.97536800	4.07880300
C	-6.50160600	8.02407400	2.66814700
H	-6.02740800	7.19336400	0.72185600
C	-6.19045300	8.06825300	4.04515600
H	-4.86675000	7.36507400	5.65250100
H	-7.27762900	9.24710900	5.50426700
C	6.44877300	3.49067300	-3.37047800
C	6.90222100	3.75995100	-4.69729800
C	7.36598400	3.48051400	-2.31640700
C	8.23225200	4.01410700	-5.00179300
H	6.16640300	3.74125800	-5.51512900
C	8.71484300	3.73618300	-2.60520900
H	7.04914900	3.30489000	-1.27850500
C	9.13642500	3.99931700	-3.92787800
H	8.55184400	4.20770000	-6.03571000
H	11.18786300	4.41563000	-4.49398700
C	4.47945800	0.26295900	6.11385700
C	4.70839900	1.17032800	7.19228200
C	5.80660500	1.07613000	8.03572100
H	3.99504800	1.99438500	7.34284300
C	5.38553500	-0.77428100	5.88215900
C	6.70387300	0.02595000	7.78444000
H	5.96120700	1.79819700	8.85009500
C	6.50092900	-0.88678500	6.72538600
H	5.22636900	-1.50918600	5.07991300

C	-6.18129800	-4.78727000	1.91735800
C	-5.76462500	-6.07219300	1.45154900
C	-6.62063900	-7.16095700	1.41481100
H	-4.72025200	-6.19682100	1.13008800
C	-7.49470700	-4.59489200	2.36019600
C	-7.94113700	-6.96880100	1.85654000
H	-6.28933600	-8.14773700	1.06218700
C	-8.35565400	-5.69997600	2.31987200
H	-7.83987000	-3.60631500	2.69509900
H	-10.36075400	-5.25587900	3.01870900
C	-4.19111400	-2.00026600	-7.08599200
C	-3.97874000	-1.78645500	-8.48235900
C	-4.60517600	-2.55107300	-9.45381600
H	-3.27071100	-1.00294800	-8.78976800
C	-5.05911200	-3.01024100	-6.65600500
C	-5.47716300	-3.56576800	-9.02365900
H	-4.42830700	-2.38669000	-10.52601800
C	-5.68773600	-3.78056600	-7.64291800
H	-5.24965100	-3.17280200	-5.58558800
H	-7.00060200	-5.30568700	-6.83478000
C	4.92153900	-5.85117500	-1.29332500
C	5.86432700	-5.70139100	-0.23080400
C	7.06329000	-6.39568500	-0.19950200
H	5.60796700	-5.02867200	0.60120200
C	5.18978800	-6.72744400	-2.35068200
C	7.33663800	-7.27256900	-1.26321500
H	7.77902700	-6.28247300	0.62684000
C	6.40393000	-7.42635000	-2.31369700
H	4.48594400	-6.83372000	-3.18845400
H	6.69736700	-8.73459900	-4.01887200
N	8.42807100	-8.08573200	-1.51326800
N	8.22849500	-8.71305400	-2.62960000
N	7.01743500	-8.33441900	-3.13618200
N	-6.57926400	-4.82104000	-7.62822700
N	-6.88797400	-5.21847300	-8.89765800
N	-6.23742400	-4.47536900	-9.73758400
N	10.86397600	4.06830400	-2.48143900
N	9.81779800	3.79547800	-1.76801400
N	10.48405200	4.19754300	-3.78778500
N	-7.59487800	8.84291300	2.43363000
N	-7.96023400	9.37588300	3.55622800
N	-7.13136600	8.92723900	4.54618400
N	-9.01073300	-7.84334600	1.93431300
N	-10.03497900	-7.20260000	2.40393100
N	-9.67084900	-5.90800800	2.64400400
N	7.53588300	-1.80794500	6.72828300
N	8.34308800	-1.51854700	7.69908400
N	7.86684600	-0.41806700	8.35419900
H	8.38385800	-0.04952300	9.15343400
H	-5.95783300	-2.85208400	3.80602800
H	4.32247900	4.74810300	-4.50971900

H	2.46483400	-6.73523100	-2.01428100
H	1.96501900	0.91707900	6.90514500
H	-3.66850400	0.65819400	-7.27826300
H	-3.94681900	7.02514700	-0.25207700
C	4.93920955	0.77446492	0.66813840
H	5.99235655	0.59483792	0.94276840
H	4.92613455	0.76643692	-0.42741560
C	4.46893155	2.06823692	1.31536640
H	4.35557155	1.93273692	2.40975540
H	3.46376755	2.35050392	0.94548640
C	4.99220244	-1.23571595	1.27136887
H	5.55368344	-0.82572995	2.12221987
H	5.63913444	-1.65049295	0.47957987
C	3.72290844	-1.80292095	1.52934487
H	3.43410344	-2.75618395	1.07505087
H	3.27017544	-1.63999695	2.51778587
C	5.44342155	3.24175992	1.10082840
H	6.46997555	2.93698792	1.40344240
H	5.49575955	3.48062792	0.01833840
C	5.02236555	4.49319192	1.87208540
H	5.72339855	5.33377692	1.69762540
H	4.01026555	4.82991792	1.56549940
H	4.98989455	4.30102092	2.96493740

P2

Ni-MFU-4l

Zn	21.36105100	9.74908900	5.99358900
Cl	20.22815500	11.11909900	4.70438800
Zn	23.24604800	7.53796200	8.09253000
N	22.67792900	10.49356400	7.34970200
C	23.12874700	11.76384400	7.54235400
N	23.32948200	9.69514700	8.19483400
C	22.77972900	12.97505900	6.91046500
C	23.45233400	14.10345900	7.33298300
H	22.01851400	13.02650100	6.11910000
Zn	21.00703600	5.47534800	9.97505600
Cl	19.65987200	4.20188400	11.15037100
N	20.24059400	6.85292800	8.69426200
C	18.95982100	7.20339400	8.38127500
N	21.06324700	7.61333000	7.97674800
C	17.71718000	6.72001200	8.83896600
C	16.59341700	7.31077200	8.29487700
H	17.63326600	5.91802200	9.58547800
Ni	25.30917800	9.48889700	10.36053600
N	23.98025400	8.13709100	11.05583400
C	23.71982300	7.71919900	12.33434700
N	23.15607800	7.48206500	10.24590700
C	24.29449600	8.04119600	13.58309400
C	23.77130200	7.40880500	14.69223900
N	20.37880400	8.45192500	7.20412100
C	19.04990700	8.23551800	7.41858700

C	17.90149900	8.83667500	6.86452100
C	16.68718000	8.36046200	7.31566100
H	17.95723100	9.63862600	6.11527300
N	24.18053200	10.38203700	8.94915200
C	24.10344300	11.69486600	8.56618800
C	24.79246200	12.85454200	8.98189300
C	24.45515400	14.03827100	8.35845500
H	25.56821500	12.84532400	9.75609000
N	22.35194100	6.66705900	10.92729000
C	22.66613600	6.77823700	12.24802000
C	22.12880500	6.13641600	13.38266900
C	22.69299800	6.46555600	14.59811400
H	21.30826200	5.40835800	13.31174000
N	22.32015900	4.59339800	8.69220400
C	22.55897800	3.28692800	8.38111300
N	23.16787600	5.34524900	7.99556800
C	21.95890600	2.09241900	8.82928300
C	22.45900500	0.92018200	8.29714800
H	21.13997100	2.08205200	9.56205400
Zn	25.35201500	5.46072200	6.04228600
Cl	26.65074200	4.19996500	4.79664600
N	24.13897700	6.82708200	5.15259200
C	23.92993500	7.14576300	3.84288600
N	23.35349500	7.60218800	5.89599000
C	24.49472600	6.64121000	2.65372700
C	24.04561600	7.20791000	1.47811100
N	23.95652300	4.58911000	7.23599600
C	23.61527800	3.28432400	7.44064300
C	24.12393500	2.08613700	6.89911000
C	23.53275900	0.91939800	7.33982800
H	24.94393700	2.06950700	6.16775200
N	22.63430400	8.41805500	5.13019700
C	22.95834100	8.17317600	3.82841900
C	22.50353900	8.75007800	2.62510900
C	23.05852400	8.25416700	1.46168500
H	21.75197100	9.55148200	2.60167700
N	26.18497900	6.68644000	7.43214000
C	27.48258800	6.89718400	7.78963300
N	25.41868100	7.45691100	8.20391300
C	28.68500400	6.35309600	7.29301500
C	29.85151900	6.80115600	7.88107500
H	28.70442400	5.61395900	6.47970100
N	26.15000300	8.16545700	9.05677600
C	27.46232500	7.84662200	8.83727400
C	28.65826700	8.28960000	9.43896500
C	29.83511300	7.76463000	8.94596500
H	28.68221200	9.01680800	10.25847600
H	25.25022400	5.84318200	2.65081200
C	23.17752600	8.31912600	-0.89850900
C	24.15467100	7.28238300	-0.88107500
C	22.74029800	8.87984400	-2.08426600

C	24.71602500	6.78340600	-2.04690100
C	23.29926300	8.38539400	-3.27666900
C	24.26777000	7.35676600	-3.24675400
H	25.46609800	5.98389900	-1.98675400
C	32.21290900	6.78068300	7.94681800
C	32.19746900	7.74441200	8.99628300
C	33.40034600	6.30388800	7.42250100
C	33.36553600	8.25705100	9.54023500
C	34.59518000	6.80849300	7.96639200
C	34.56618800	7.76693000	9.00422900
H	33.30822000	9.00361400	10.34250700
C	14.32907400	8.47360100	7.22041900
C	14.23493300	7.43418800	8.19019600
C	13.20352100	9.06777900	6.66981300
C	13.01104100	6.96594900	8.63101000
C	11.96455900	8.58795400	7.12150800
C	11.85853600	7.55769200	8.08294300
H	12.95699000	6.16424000	9.37889500
C	22.37937300	-1.44049900	8.19855600
C	23.44270600	-1.44007900	7.25029200
C	21.79915700	-2.61800000	8.63271800
C	23.94946900	-2.61491300	6.71533500
C	22.30105200	-3.81936600	8.10018800
C	23.35615400	-3.80628300	7.16019100
H	24.76987600	-2.56779400	5.98722000
O	31.03663700	6.29236300	7.42274500
O	31.00827800	8.19949600	9.51356300
H	33.39406100	5.56148000	6.61395000
N	35.91282900	6.52864000	7.65594700
N	35.89379800	7.99749200	9.24580700
N	36.67937500	7.24044200	8.42245600
O	21.89753600	-0.25673300	8.71196000
O	24.00804400	-0.26215300	6.82937100
H	20.98062700	-2.59991800	9.36393800
N	21.93225500	-5.13040800	8.33658000
N	23.54755000	-5.13567800	6.89569200
N	22.67919400	-5.90766100	7.61563900
C	23.82012000	7.10987300	17.03556300
C	22.74776400	6.17585500	16.94222000
C	24.39467600	7.44776500	18.25187800
C	22.22759700	5.55938100	18.06529100
C	23.86203300	6.81824900	19.38734500
C	22.79926700	5.89038600	19.30714800
H	21.40130700	4.84236700	17.97501200
O	22.19708700	5.85937400	15.72046900
O	24.32658800	7.71350200	15.91140500
H	25.21865600	8.17290200	18.27812800
N	24.12743600	6.86516200	20.72950700
N	22.49901600	5.44683800	20.58148100
N	23.29402600	6.03194100	21.42237500
H	25.12226400	8.74963700	13.70004800

O	22.63799600	8.79379900	0.27647900
O	24.57815700	6.73618700	0.30480500
H	21.98671300	9.67800700	-2.07923000
N	24.55180900	7.16460500	-4.57201000
N	23.81666900	8.00794800	-5.35718900
N	23.06698000	8.73946200	-4.59248100
O	15.37187100	6.86352500	8.71870800
H	13.32271100	9.86564800	5.92507300
O	15.55228300	8.92717100	6.79345300
N	10.65719500	8.88682700	6.84708200
N	10.52009900	7.30745900	8.32091900
N	9.81171000	8.10297200	7.58116200
C	23.80434300	16.43208300	7.14352200
C	24.80272300	16.36679600	8.15849100
C	23.47097500	17.62801800	6.53481200
C	25.48809000	17.49412800	8.58651500
C	24.15695000	18.78119900	6.95690600
C	25.14475300	18.70426400	7.96442800
H	26.24931200	17.39874600	9.37194200
O	23.14007300	15.29608800	6.73830300
O	25.12356900	15.17193800	8.75330400
H	22.69946800	17.65997800	5.75458400
N	24.04508500	20.09537600	6.54313200
N	24.88477800	20.81600000	7.21929100
N	25.56193500	20.00257100	8.08450200
H	24.82466400	7.41121900	21.23642100
H	10.26896900	9.57745300	6.20385000
H	24.21558700	-5.58460700	6.26833800
H	36.33311100	8.62294100	9.92196300
H	26.26852100	20.40481600	8.70111900
H	25.20230800	6.51151900	-5.00989000
C	25.41713800	10.79778500	11.84475900
H	24.57632300	10.60025000	12.54219800
C	26.78081500	10.69300400	12.54617200
H	25.26122100	11.83381400	11.47648900
C	27.93296000	11.23483500	11.69144700
H	27.82202200	10.84545100	10.65063300
H	27.82942700	12.33858900	11.59005100
C	29.32743100	10.89129000	12.21775600
H	29.40179600	9.78782800	12.36090600
H	29.45540300	11.32513400	13.23493000
C	30.47391200	11.35159400	11.31352500
H	30.35467100	10.89298500	10.30735500
H	30.40077000	12.45040900	11.15610600
C	31.85199700	10.99690700	11.87227400
H	31.94613100	9.90068000	12.02069100
H	32.66743100	11.32231200	11.19437100
H	32.02629500	11.47682100	12.85776700
H	26.77841300	11.23493100	13.52340600
H	27.00876200	9.63264000	12.81438000

Ni-CFA-1

Zn	-0.65066200	2.94490400	-2.69810900
Cl	-0.90946300	4.54964600	-4.17443900
Zn	-0.22969200	0.30128000	-0.30881200
N	1.21051500	2.38067900	-2.11383800
C	2.43472400	2.81912800	-2.52346600
N	1.40875400	1.40917300	-1.21255600
C	2.83273800	3.80216500	-3.45368800
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90790000	1.20907800	2.76740500
Cl	-2.93116700	1.77532300	4.62705200
N	-1.93757200	2.48279500	1.18351800
C	-2.52180300	3.70875200	1.03041100
N	-1.32705500	2.17420200	0.04391200
C	-3.28517600	4.49134500	1.91600000
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.26334200	-0.23165700	0.33808900
N	1.97151400	0.17906500	1.84741100
C	2.24953900	0.36729400	3.19036900
N	0.66645400	0.40998500	1.65491300
C	3.39343300	0.15232100	3.97730800
C	3.27563500	0.32177600	5.35402400
N	-1.48173300	3.14067900	-0.85426900
C	-2.22727700	4.13298300	-0.28494500
C	-2.68118300	5.37805100	-0.76767300
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69256000	1.19316900	-0.99535400
C	3.38403700	2.05247400	-1.80939100
C	4.76566800	2.21598500	-2.01818300
C	5.17329100	3.18509500	-2.93035200
H	5.49198500	1.57922400	-1.49265700
N	0.07379300	0.77749600	2.79043500
C	1.01305500	0.72852900	3.77005800
C	0.88044100	0.91425000	5.16240000
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48728700	-0.45877100	1.75237000
C	-3.45841500	-1.38128900	2.01243800
N	-1.88972200	-0.80077600	0.61587300
C	-4.39762400	-1.50246100	3.05748300
C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.70044600	-2.72733500	-1.60285900
Cl	-2.64732800	-4.55160100	-2.38471500
N	-1.73402400	-1.02968600	-2.72085200
C	-2.26408100	-0.77700400	-3.95371900
N	-1.21564800	0.10258400	-2.25791800
C	-2.92036300	-1.61553000	-4.87284000

C	-3.35131100	-1.04003100	-6.06579400
N	-2.42155700	-1.90894000	0.11381300
C	-3.41786300	-2.31659200	0.95387700
C	-4.31060000	-3.40170300	0.87962800
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37561400	1.09162200	-3.12979900
C	-2.03121000	0.59171700	-4.21779500
C	-2.46163500	1.18452300	-5.42315900
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27213000	-2.70121600	-1.14004400
C	1.26075900	-3.63213200	-1.23688200
N	0.82041300	-1.57869900	-0.67013800
C	1.24385400	-4.97589900	-1.66655900
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12219700	-1.72895700	-0.45994500
C	2.45777300	-3.01985100	-0.80024500
C	3.68415100	-3.70928700	-0.78606000
C	3.67974000	-5.03712900	-1.20460000
H	4.61466300	-3.21412700	-0.48495100
H	-3.05604700	-2.68397400	-4.64962800
H	4.19926300	-0.53508100	3.73825100
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700

C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400

H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	5.03741400	0.26759300	1.05918900
H	5.63457800	0.79509700	0.28427700
H	4.93640000	0.97294500	1.91135700
C	5.76110300	-1.01890200	1.47448400
H	5.88162600	-1.69241800	0.59329600
C	7.15845700	-0.79920100	2.08491900
H	7.77688100	-0.23499000	1.35048200
H	7.06033200	-0.13354700	2.97044800
C	7.87473600	-2.09990000	2.46839600
H	7.34928000	-2.57329700	3.32927000
H	7.78511200	-2.81843200	1.62181400
H	5.15172600	-1.60919200	2.20126200
C	9.36142600	-1.93009500	2.81539800
H	9.80438400	-2.93644000	2.97834400
H	9.88930000	-1.50689200	1.93118300
C	9.63033800	-1.05964000	4.04487600
H	10.71586200	-0.99636100	4.26227700
H	9.26361900	-0.02180400	3.90399000
H	9.12939000	-1.47813500	4.94109300

βH^A

Ni-MFU-4l

Zn	21.26439200	9.80104100	5.92629800
Cl	20.06115400	11.08522000	4.61110100
Zn	23.22482800	7.66805100	8.07555800
N	22.52048800	10.62622200	7.28759500
C	22.85376600	11.90101500	7.61964500
N	23.22572600	9.81897800	8.07637200
C	22.40371600	13.12225800	7.07732400
C	22.94287800	14.27123900	7.62280700
H	21.67161600	13.17040700	6.25908000
Zn	21.03563500	5.58085500	10.01666300
Cl	19.70540200	4.28471800	11.18919400
N	20.24544000	6.91182200	8.69342200
C	18.95637100	7.22546800	8.38026200
N	21.04499800	7.67824400	7.95619200
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66781400	5.92669900	9.61077100
Ni	25.19249500	9.63887300	10.23712100
N	23.91087900	8.34599700	11.02044300
C	23.63101600	8.03855700	12.32620300
N	23.09214000	7.63721200	10.23834500
C	24.16437900	8.47598800	13.55575500

C	23.63165600	7.90626900	14.69382100
N	20.33772900	8.48535200	7.17066900
C	19.01672100	8.24104300	7.39762800
C	17.85133600	8.80037700	6.83529300
C	16.65118000	8.29983100	7.29796700
H	17.88463200	9.58818200	6.06967500
N	24.02788400	10.51606900	8.89597900
C	23.79898500	11.85166400	8.66984600
C	24.33789900	13.02694600	9.22898200
C	23.90451800	14.22034900	8.68926100
H	25.15352200	13.06988600	9.94547200
N	22.31102900	6.83944200	10.96321700
C	22.61198000	7.05901800	12.27056400
C	22.06943800	6.47883200	13.43552500
C	22.59041200	6.91662500	14.63694700
H	21.27660600	5.71839200	13.40136300
N	22.38614800	4.72237800	8.75127100
C	22.66029100	3.41765800	8.46707600
N	23.20358300	5.48071200	8.02624300
C	22.09628400	2.21746600	8.94586100
C	22.62174800	1.04783200	8.43285600
H	21.28320700	2.20140000	9.68518900
Zn	25.37575400	5.61008600	6.05432300
Cl	26.69495200	4.35084200	4.82546600
N	24.12770300	6.93361500	5.14586800
C	23.92462400	7.24378200	3.83402300
N	23.32036700	7.69616600	5.87819400
C	24.50789600	6.74361500	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00626700	4.73091100	7.27520800
C	23.70625700	3.42283000	7.51470400
C	24.24096000	2.22720600	6.99294100
C	23.68565700	1.05498700	7.46445000
H	25.05315300	2.21699300	6.25272100
N	22.59351200	8.49713800	5.10388700
C	22.93495900	8.25376100	3.80676600
C	22.47909500	8.81547600	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71025800	9.60011900	2.56309700
N	26.19068800	6.86246100	7.42762700
C	27.47473800	7.09680700	7.81543600
N	25.39660200	7.62198300	8.18233100
C	28.69606700	6.55976200	7.35869000
C	29.83970100	7.02435300	7.97882700
H	28.74830500	5.81601700	6.55109100
N	26.09232400	8.36266900	9.04051400
C	27.42224500	8.05140400	8.85742500
C	28.58975000	8.50206100	9.50290200
C	29.78335200	7.98755700	9.04355900
H	28.59846900	9.22820400	10.32363600
H	25.27725400	5.95892000	2.65934000

C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53109700	6.08357600	-1.97703600
C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19650900	9.15985000	10.63101000
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700
C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98579600	6.04170800	9.40977800
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00225500	-2.42630400	6.17336600
O	31.04330900	6.52965100	7.55274100
O	30.93540500	8.43361100	9.64449300
H	33.42610700	5.73163600	6.89594100
N	35.89879200	6.62663400	8.09905900
N	35.81985500	8.08939700	9.69222100
N	36.63482700	7.31287100	8.91678600
O	22.09512300	-0.13452700	8.87738200
O	24.18709100	-0.12435500	6.97387300
H	21.24697700	-2.48629900	9.58757400
N	22.25604700	-5.01225200	8.60433500
N	23.85722600	-5.00567800	7.14822100
N	23.01652300	-5.78493100	7.89273700
C	23.63027400	7.76263300	17.05262700
C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27575600	5.46733300	18.08364000
O	22.08380100	6.37312100	15.78725300
O	24.13837300	8.31631900	15.90315500
H	24.96131000	8.95228300	18.25436600
N	23.86404000	7.75833100	20.76015500

N	22.29189200	6.27373500	20.66894800
N	23.04621400	6.93905400	21.48732400
H	24.95824500	9.22703900	13.63857400
O	22.63075600	8.84933200	0.24881600
O	24.60882400	6.82827900	0.30315900
H	21.98432500	9.71164600	-2.11589600
N	24.61804400	7.23671700	-4.57534600
N	23.87445100	8.06289900	-5.37075100
N	23.10459100	8.78328000	-4.61561200
O	15.37926900	6.79418800	8.73182300
H	13.24482700	9.68605100	5.88625200
O	15.50010000	8.82560500	6.76759400
N	10.60828600	8.65194800	6.83193300
N	10.51683800	7.09773400	8.33530400
N	9.78554300	7.85924100	7.58218600
C	23.05992300	16.63156900	7.64155300
C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30567400	17.64348800	10.05242900
O	22.53411200	15.47487300	7.11194800
O	24.44650600	15.37643000	9.19824500
H	21.89098500	17.85675200	6.30368700
N	22.94733900	20.33803400	7.34842300
N	23.68143600	21.07888000	8.11895200
N	24.40377400	20.26630700	8.94763700
H	24.52931700	8.36069900	21.24579500
H	10.20029100	9.31932200	6.17649800
H	24.53094600	-5.45014700	6.52375700
H	36.23323100	8.69958400	10.39805900
H	25.04051300	20.68321200	9.62737600
H	25.28432300	6.59395800	-5.00472000
C	24.87192300	10.95443400	11.58595500
H	24.45065100	11.89804300	11.21561300
C	26.35558600	10.83953900	11.67697900
H	26.67803400	9.87983100	11.05621100
H	24.27526000	10.58315600	12.43211600
C	27.20835700	12.01245700	11.16784400
H	28.28489000	11.74017900	11.21889900
H	26.99779800	12.16318600	10.08764300
C	26.96872700	13.32441900	11.92406200
H	27.31314400	13.22203800	12.97738500
H	25.87364600	13.51282000	11.99314900
H	26.69323900	10.49842400	12.68178000
C	27.63526600	14.53799700	11.26755600
H	28.73705900	14.38748300	11.23909900
H	27.31033600	14.59329200	10.20469200
C	27.30231700	15.85818300	11.96266900
H	27.62735000	15.85603100	13.02390300

H	27.79534900	16.71743700	11.46454800
H	26.20736400	16.04285700	11.95268400

Ni-CFA-1

Zn	-0.64787000	2.94410800	-2.69662200
Cl	-0.90946800	4.54967100	-4.17442500
Zn	-0.21530300	0.29927800	-0.30407600
N	1.21037700	2.38047400	-2.11399800
C	2.43465600	2.81911900	-2.52338000
N	1.40934500	1.40811400	-1.21366400
C	2.83273800	3.80217100	-3.45368100
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90231100	1.20830500	2.76842300
Cl	-2.93117300	1.77531200	4.62705200
N	-1.93756600	2.48282800	1.18351700
C	-2.52180700	3.70875000	1.03041000
N	-1.32709600	2.17420200	0.04396100
C	-3.28518000	4.49134300	1.91599900
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.18553800	-0.20990700	0.29622400
N	1.96668500	0.14495600	1.85416200
C	2.24949600	0.36694000	3.19012900
N	0.66648300	0.40965700	1.65467800
C	3.39344600	0.15246800	3.97732900
C	3.27564000	0.32179400	5.35402200
N	-1.48178600	3.14074500	-0.85420100
C	-2.22726400	4.13298700	-0.28493500
C	-2.68119100	5.37804700	-0.76767600
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69592600	1.16408500	-1.02511400
C	3.38425700	2.05324200	-1.80900600
C	4.76568200	2.21611800	-2.01799000
C	5.17328800	3.18503000	-2.93042200
H	5.49198100	1.57914100	-1.49275100
N	0.07381000	0.77748100	2.79045200
C	1.01308400	0.72857200	3.77008100
C	0.88045300	0.91430400	5.16239400
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48727900	-0.45874900	1.75236100
C	-3.45840800	-1.38129500	2.01244100
N	-1.88973800	-0.80077700	0.61586000
C	-4.39762200	-1.50246300	3.05748500
C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.69815200	-2.72664200	-1.60184600
Cl	-2.64731600	-4.55158100	-2.38474900

N	-1.73403800	-1.02963600	-2.72090500
C	-2.26408700	-0.77699900	-3.95371600
N	-1.21563700	0.10266600	-2.25791800
C	-2.92036700	-1.61552900	-4.87283800
C	-3.35131100	-1.04003100	-6.06579400
N	-2.42150600	-1.90894500	0.11375600
C	-3.41786700	-2.31659000	0.95387300
C	-4.31059500	-3.40170800	0.87963200
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37557700	1.09169700	-3.12973500
C	-2.03120600	0.59171900	-4.21779800
C	-2.46163000	1.18452200	-5.42316200
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27226000	-2.70141700	-1.13978400
C	1.26084200	-3.63225300	-1.23694200
N	0.81971300	-1.57843800	-0.66898100
C	1.24387400	-4.97586700	-1.66666000
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12665600	-1.71760200	-0.45688000
C	2.45758700	-3.01919000	-0.80019400
C	3.68417100	-3.70925800	-0.78636800
C	3.67973900	-5.03713000	-1.20459700
H	4.61464100	-3.21416400	-0.48482100
H	-3.05604700	-2.68397400	-4.64962800
H	4.19925000	-0.53510100	3.73826400
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400

H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700
C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400

N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400
H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	4.60597000	0.82712300	1.04903000
H	4.96991900	1.64076800	0.40126300
H	4.37882400	1.19802200	2.06214600
C	5.32163300	-0.47865500	0.94905800
H	4.56487700	-1.28030900	0.52844900
C	6.56453100	-0.53322500	0.04831200
H	6.28168700	-0.24204800	-0.98591900
H	7.27758700	0.24261000	0.40330400
C	7.27174100	-1.88881700	0.01535700
H	7.54910700	-2.18710500	1.05194400
H	6.56894900	-2.67387100	-0.34339400
H	5.54003600	-0.91432900	1.94829900
C	8.52134700	-1.90151100	-0.87072800
H	8.23534100	-1.59197500	-1.90078200
H	9.22811800	-1.12112900	-0.51110900
C	9.22189000	-3.25958100	-0.91527400
H	10.12578200	-3.23230400	-1.55578700
H	9.54220900	-3.58171300	0.09772000
H	8.55151300	-4.04937100	-1.31267200

TS-βH^A

Ni-MFU-4l

Zn	21.26255600	9.79821600	5.92371700
Cl	20.06115400	11.08522000	4.61110100
Zn	23.22689600	7.66086600	8.06750300
N	22.52048800	10.62622200	7.28759500
C	22.85376600	11.90101500	7.61964500
N	23.22572600	9.81897800	8.07637200
C	22.40371600	13.12225800	7.07732400
C	22.94287800	14.27123900	7.62280700
H	21.67161600	13.17040700	6.25908000
Zn	21.03429500	5.57804100	10.01374700
Cl	19.70540200	4.28471800	11.18919400
N	20.24544000	6.91182200	8.69342200
C	18.95637100	7.22546800	8.38026200
N	21.04499800	7.67824400	7.95619200
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66781400	5.92669900	9.61077100
Ni	25.20733700	9.68046600	10.37500000

N	23.89364800	8.36204100	11.02308400
C	23.63101600	8.03855700	12.32620300
N	23.09214000	7.63721200	10.23834500
C	24.16437900	8.47598800	13.55575500
C	23.63165600	7.90626900	14.69382100
N	20.33772900	8.48535200	7.17066900
C	19.01672100	8.24104300	7.39762800
C	17.85133600	8.80037700	6.83529300
C	16.65118000	8.29983100	7.29796700
H	17.88463200	9.58818200	6.06967500
N	24.00317300	10.51409500	8.91681900
C	23.79898500	11.85166400	8.66984600
C	24.33789900	13.02694600	9.22898200
C	23.90451800	14.22034900	8.68926100
H	25.15352200	13.06988600	9.94547200
N	22.31102900	6.83944200	10.96321700
C	22.61198000	7.05901800	12.27056400
C	22.06943800	6.47883200	13.43552500
C	22.59041200	6.91662500	14.63694700
H	21.27660600	5.71839200	13.40136300
N	22.38614800	4.72237800	8.75127100
C	22.66029100	3.41765800	8.46707600
N	23.20358300	5.48071200	8.02624300
C	22.09628400	2.21746600	8.94586100
C	22.62174800	1.04783200	8.43285600
H	21.28320700	2.20140000	9.68518900
Zn	25.37886200	5.61025100	6.05553800
Cl	26.69495200	4.35084200	4.82546600
N	24.12770300	6.93361500	5.14586800
C	23.92462400	7.24378200	3.83402300
N	23.32036700	7.69616600	5.87819400
C	24.50789600	6.74361500	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00626700	4.73091100	7.27520800
C	23.70625700	3.42283000	7.51470400
C	24.24096000	2.22720600	6.99294100
C	23.68565700	1.05498700	7.46445000
H	25.05315300	2.21699300	6.25272100
N	22.59351200	8.49713800	5.10388700
C	22.93495900	8.25376100	3.80676600
C	22.47909500	8.81547600	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71025800	9.60011900	2.56309700
N	26.19068800	6.86246100	7.42762700
C	27.47473800	7.09680700	7.81543600
N	25.39660200	7.62198300	8.18233100
C	28.69606700	6.55976200	7.35869000
C	29.83970100	7.02435300	7.97882700
H	28.74830500	5.81601700	6.55109100
N	26.09639100	8.35580400	9.03938900
C	27.42224500	8.05140400	8.85742500

C	28.58975000	8.50206100	9.50290200
C	29.78335200	7.98755700	9.04355900
H	28.59846900	9.22820400	10.32363600
H	25.27725400	5.95892000	2.65934000
C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53109700	6.08357600	-1.97703600
C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19650900	9.15985000	10.63101000
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700
C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98579600	6.04170800	9.40977800
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00225500	-2.42630400	6.17336600
O	31.04330900	6.52965100	7.55274100
O	30.93540500	8.43361100	9.644449300
H	33.42610700	5.73163600	6.89594100
N	35.89879200	6.62663400	8.09905900
N	35.81985500	8.08939700	9.69222100
N	36.63482700	7.31287100	8.91678600
O	22.09512300	-0.13452700	8.87738200
O	24.18709100	-0.12435500	6.97387300
H	21.24697700	-2.48629900	9.58757400
N	22.25604700	-5.01225200	8.60433500
N	23.85722600	-5.00567800	7.14822100
N	23.01652300	-5.78493100	7.89273700
C	23.63027400	7.76263300	17.05262700
C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27575600	5.46733300	18.08364000

O	22.08380100	6.37312100	15.78725300
O	24.13837300	8.31631900	15.90315500
H	24.96131000	8.95228300	18.25436600
N	23.86404000	7.75833100	20.76015500
N	22.29189200	6.27373500	20.66894800
N	23.04621400	6.93905400	21.48732400
H	24.95824500	9.22703900	13.63857400
O	22.63075600	8.84933200	0.24881600
O	24.60882400	6.82827900	0.30315900
H	21.98432500	9.71164600	-2.11589600
N	24.61804400	7.23671700	-4.57534600
N	23.87445100	8.06289900	-5.37075100
N	23.10459100	8.78328000	-4.61561200
O	15.37926900	6.79418800	8.73182300
H	13.24482700	9.68605100	5.88625200
O	15.50010000	8.82560500	6.76759400
N	10.60828600	8.65194800	6.83193300
N	10.51683800	7.09773400	8.33530400
N	9.78554300	7.85924100	7.58218600
C	23.05992300	16.63156900	7.64155300
C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30567400	17.64348800	10.05242900
O	22.53411200	15.47487300	7.11194800
O	24.44650600	15.37643000	9.19824500
H	21.89098500	17.85675200	6.30368700
N	22.94733900	20.33803400	7.34842300
N	23.68143600	21.07888000	8.11895200
N	24.40377400	20.26630700	8.94763700
H	24.52931700	8.36069900	21.24579500
H	10.20029100	9.31932200	6.17649800
H	24.53094600	-5.45014700	6.52375700
H	36.23323100	8.69958400	10.39805900
H	25.04051300	20.68321200	9.62737600
H	25.28432300	6.59395800	-5.00472000
C	24.51883900	11.27643600	11.96653900
H	24.11032500	12.04276300	11.30146900
C	25.89759800	10.97555900	12.02746400
H	26.40401500	9.48321700	11.39035100
H	23.81280900	10.84010800	12.68481700
C	26.94086300	11.87148400	11.35712000
H	27.94801000	11.42350300	11.48651300
H	26.78197000	11.89375300	10.25440400
C	26.93171000	13.31491600	11.88502900
H	27.19964500	13.31399500	12.96475200
H	25.89402600	13.71256200	11.84542700
H	26.25951100	10.52705300	12.96994100
C	27.86062100	14.25376100	11.10986500

H	28.90928000	13.89062600	11.18721200
H	27.60380800	14.20135600	10.02782300
C	27.77095400	15.70568700	11.58009600
H	28.03900100	15.80396200	12.65256900
H	28.44763800	16.36696400	11.00260000
H	26.73641200	16.09150300	11.46117800

Ni-CFA-1

Zn	-0.65037500	2.94397500	-2.69666900
Cl	-0.90946800	4.54967100	-4.17442500
Zn	-0.21715000	0.30093500	-0.30060800
N	1.21037700	2.38047400	-2.11399800
C	2.43465600	2.81911900	-2.52338000
N	1.40934500	1.40811400	-1.21366400
C	2.83273800	3.80217100	-3.45368100
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90011300	1.20756900	2.77004000
Cl	-2.93117300	1.77531200	4.62705200
N	-1.93756600	2.48282800	1.18351700
C	-2.52180700	3.70875000	1.03041000
N	-1.32709600	2.17420200	0.04396100
C	-3.28518000	4.49134300	1.91599900
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.27376900	-0.29665600	0.30248300
N	1.96713300	0.17224800	1.84512800
C	2.24949600	0.36694000	3.19012900
N	0.66648300	0.40965700	1.65467800
C	3.39344600	0.15246800	3.97732900
C	3.27564000	0.32179400	5.35402200
N	-1.48178600	3.14074500	-0.85420100
C	-2.22726400	4.13298700	-0.28493500
C	-2.68119100	5.37804700	-0.76767600
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69541000	1.17281300	-1.00464200
C	3.38425700	2.05324200	-1.80900600
C	4.76568200	2.21611800	-2.01799000
C	5.17328800	3.18503000	-2.93042200
H	5.49198100	1.57914100	-1.49275100
N	0.07381000	0.77748100	2.79045200
C	1.01308400	0.72857200	3.77008100
C	0.88045300	0.91430400	5.16239400
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48727900	-0.45874900	1.75236100
C	-3.45840800	-1.38129500	2.01244100
N	-1.88973800	-0.80077700	0.61586000
C	-4.39762200	-1.50246300	3.05748500
C	-5.26727600	-2.57364300	2.97938200

H	-4.41867500	-0.77915700	3.88583600
Zn	-1.69963600	-2.72638200	-1.60145000
Cl	-2.64731600	-4.55158100	-2.38474900
N	-1.73403800	-1.02963600	-2.72090500
C	-2.26408700	-0.77699900	-3.95371600
N	-1.21563700	0.10266600	-2.25791800
C	-2.92036700	-1.61552900	-4.87283800
C	-3.35131100	-1.04003100	-6.06579400
N	-2.42150600	-1.90894500	0.11375600
C	-3.41786700	-2.31659000	0.95387300
C	-4.31059500	-3.40170800	0.87963200
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37557700	1.09169700	-3.12973500
C	-2.03120600	0.59171900	-4.21779800
C	-2.46163000	1.18452200	-5.42316200
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27226000	-2.70141700	-1.13978400
C	1.26084200	-3.63225300	-1.23694200
N	0.81971300	-1.57843800	-0.66898100
C	1.24387400	-4.97586700	-1.66666000
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12977400	-1.72016500	-0.47029500
C	2.45758700	-3.01919000	-0.80019400
C	3.68417100	-3.70925800	-0.78636800
C	3.67973900	-5.03713000	-1.20459700
H	4.61464100	-3.21416400	-0.48482100
H	-3.05604700	-2.68397400	-4.64962800
H	4.19925000	-0.53510100	3.73826400
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200

C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700
C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000

N	-9.10673100	-7.65550300	1.85159000
N	10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400
H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	4.84317400	0.68542200	0.97064000
H	5.02292400	1.58667100	0.36953100
H	4.74600400	0.88026200	2.04967300
C	5.30526900	-0.60021800	0.53878100
H	3.89865000	-1.40077100	0.99633800
C	6.06509300	-0.88287000	-0.75857400
H	5.37518500	-1.18801100	-1.57375500
H	6.53963800	0.05784200	-1.11221200
C	7.16141000	-1.94211500	-0.59853400
H	7.89354700	-1.60014600	0.16669300
H	6.72186800	-2.87971300	-0.19004700
H	5.63419700	-1.26987100	1.36008000
C	7.88909100	-2.26210200	-1.90696400
H	7.14200400	-2.61000900	-2.65523400
H	8.31620400	-1.32249300	-2.32350200
C	8.99013300	-3.31108000	-1.75102200
H	9.50048200	-3.51363800	-2.71372400
H	9.76326800	-2.98001900	-1.02678600
H	8.57913400	-4.27348000	-1.38263800

PβH^A

Ni-MFU-4l

Zn	21.27417900	9.78821900	6.04401700
Cl	20.13871400	11.17042500	4.76471300
Zn	23.17686100	7.57663500	8.11471700
N	22.62211900	10.55043400	7.37359700
C	23.12938700	11.80615400	7.53222900
N	23.26600000	9.73765800	8.21394900
C	22.82294000	13.02238800	6.88298700
C	23.56988800	14.13090600	7.26133400
H	22.04374800	13.09661200	6.11130000
Zn	20.96670900	5.50596700	10.00814000
Cl	19.63486400	4.22338000	11.19691400
N	20.15370000	6.88564500	8.74257200
C	18.86596800	7.24177900	8.45607200
N	20.96722300	7.64822600	8.01469600
C	17.62711900	6.76211700	8.93478600
C	16.48916100	7.36702200	8.41326800

H	17.55212200	5.95586600	9.67760000
Ni	25.39597987	9.45471542	10.37292876
N	23.97776400	8.12882600	11.05390100
C	23.78549100	7.67504500	12.33388200
N	23.12085900	7.49488800	10.26719000
C	24.43409200	7.95426600	13.55788400
C	23.94969400	7.30516300	14.68599100
N	20.27369600	8.49658500	7.25835300
C	18.94434800	8.28691600	7.49284500
C	17.78697400	8.89922300	6.96422000
C	16.57062000	8.42415800	7.43817900
H	17.83238900	9.70574800	6.21928500
N	24.18063500	10.39587200	8.93913000
C	24.13473600	11.70782800	8.53671800
C	24.90020300	12.84079200	8.90023700
C	24.60345000	14.03544800	8.25577800
H	25.70980800	12.81037600	9.63894900
N	22.32943900	6.67705100	10.96537000
C	22.70237600	6.75195300	12.27561800
C	22.20960000	6.09419200	13.42414600
C	22.84457300	6.38704500	14.62468400
H	21.37316400	5.38239700	13.38058000
N	22.25959800	4.60537600	8.70237300
C	22.50230600	3.29769200	8.39086400
N	23.10029400	5.36258400	8.00045200
C	21.91095300	2.09704700	8.84151800
C	22.41767900	0.92061100	8.30147700
H	21.09672200	2.08040800	9.57934200
Zn	25.27956700	5.52027100	6.04869300
Cl	26.57850600	4.26672500	4.78973900
N	24.05682800	6.87957400	5.14378100
C	23.84212800	7.20202600	3.83403400
N	23.26845500	7.64681300	5.89452300
C	24.40441000	6.70581000	2.63734200
C	23.94384700	7.27979900	1.45913000
N	23.89047200	4.61183800	7.23503700
C	23.56003300	3.30228600	7.43820900
C	24.07295300	2.10554800	6.89133000
C	23.48729100	0.92718400	7.33661200
H	24.88886600	2.09404600	6.15536200
N	22.53968800	8.46400900	5.13699500
C	22.85843100	8.23086000	3.82942300
C	22.39452000	8.81245600	2.62905200
C	22.95003700	8.32255700	1.45273200
H	21.63907700	9.61034900	2.61302300
N	26.13995800	6.73274500	7.44018600
C	27.44140600	6.92638600	7.80450400
N	25.37414000	7.50348700	8.21600000
C	28.64762900	6.37675900	7.31611100
C	29.81805900	6.80955500	7.92909300
H	28.67207600	5.64667900	6.49491300

N	26.11287200	8.20807400	9.06865800
C	27.42094300	7.86963500	8.86935300
C	28.61282000	8.29932900	9.49114100
C	29.79819200	7.76188800	9.00710900
H	28.62451700	9.01763600	10.31909400
H	25.16391200	5.91171100	2.62611200
C	23.05653800	8.40203200	-0.91047500
C	24.04187700	7.36664400	-0.90300600
C	22.60836400	8.97012900	-2.09780800
C	24.60323100	6.87365800	-2.08089500
C	23.16471600	8.48423800	-3.29959100
C	24.14534600	7.45257900	-3.27857600
H	25.35735500	6.07748000	-2.02778200
C	32.17963900	6.72864800	8.05308500
C	32.16060700	7.67756200	9.12223100
C	33.37432300	6.21290000	7.56233100
C	33.33235900	8.13520700	9.72510400
C	34.56996300	6.66207200	8.16072100
C	34.53648700	7.60804600	9.22374000
H	33.27118400	8.86553200	10.54214900
C	14.20906800	8.55311200	7.38887400
C	14.12695700	7.50463400	8.35670000
C	13.07023800	9.16155800	6.86138700
C	12.90208700	7.03882100	8.82141100
C	11.83419600	8.68561200	7.33562200
C	11.73879200	7.64236700	8.29946200
H	12.85934000	6.23251100	9.56510600
C	22.34825700	-1.44310900	8.20023000
C	23.40945000	-1.43541600	7.24278600
C	21.77274200	-2.63090000	8.63762300
C	23.92157800	-2.61344600	6.69918600
C	22.27765200	-3.83285100	8.09883100
C	23.33499500	-3.81159200	7.14593600
H	24.73749900	-2.56009800	5.96648500
O	31.00505000	6.29653600	7.47715400
O	30.96978400	8.17364600	9.59773600
H	33.36923400	5.48492500	6.74070900
N	35.88635000	6.33964200	7.89809000
N	35.86155700	7.77860200	9.51697800
N	36.64884900	7.00676500	8.70796400
O	21.86532500	-0.26091100	8.71801600
O	23.96580300	-0.25234400	6.82224300
H	20.95842400	-2.61645700	9.37364600
N	21.91960900	-5.14563000	8.33142000
N	23.52774700	-5.13936800	6.88031100
N	22.66662200	-5.91708900	7.60391500
C	24.11995100	6.93696300	17.01675400
C	23.01717000	6.02892500	16.95668300
C	24.77492400	7.22344900	18.21469900
C	22.54319600	5.38608200	18.09501900
C	24.29033100	6.56956300	19.36226100

C	23.19318700	5.66384900	19.31569100
H	21.69519600	4.69212000	18.02877600
O	22.39152100	5.76561800	15.75796700
O	24.57470400	7.56466300	15.88289800
H	25.61752900	7.92733600	18.21487200
N	24.62901600	6.56454200	20.68745200
N	22.95754000	5.19026000	20.59081900
N	23.81437500	5.72950700	21.40144000
H	25.29424500	8.62983500	13.63803600
O	22.52147600	8.86643600	0.27144700
O	24.47270800	6.81730500	0.27954100
H	21.85090200	9.76453000	-2.08316800
N	24.42090700	7.27200300	-4.60605000
N	23.67754700	8.11644500	-5.38332900
N	22.92750100	8.84092900	-4.61189400
O	15.27235200	6.92433600	8.85759200
H	13.18069700	9.96340000	6.11958200
O	15.42809300	9.00062300	6.94179900
N	10.52354000	8.99139500	7.09208600
N	10.40443400	7.40246800	8.55940700
N	9.68751200	8.20782600	7.83833200
C	24.04195200	16.43380000	6.99722300
C	25.07493000	16.33713600	7.98104800
C	23.75356000	17.63751400	6.36348200
C	25.84359400	17.43983700	8.35430000
C	24.52062800	18.76362600	6.72836700
C	25.54648100	18.65423200	7.70910800
H	26.62652200	17.32037800	9.11469300
O	23.30044400	15.32622500	6.64919600
O	25.34619600	15.14043100	8.59842100
H	22.95668500	17.69197300	5.61043100
N	24.47175900	20.06997200	6.28476100
N	25.37626100	20.75740700	6.91041800
N	26.03807100	19.92897000	7.77426400
H	25.36728000	7.07592900	21.17202900
H	10.12491800	9.68793000	6.46161500
H	24.19340900	-5.58598600	6.24870400
H	36.30045500	8.37252400	10.22130100
H	26.78880700	20.30781700	8.35243100
H	25.07178600	6.62516900	-5.05269300
C	25.34983887	10.95160842	11.66862976
H	24.97357687	10.58382842	12.63657976
C	26.68109900	10.74325000	11.33398400
H	24.77704187	11.79756442	11.25851776
C	27.61212400	11.61686600	10.49853500
H	27.60437100	11.31260900	9.42945900
H	27.26401600	12.67233800	10.51507500
C	29.05932000	11.59821400	11.01312100
H	29.38955600	10.54799000	11.17486500
H	29.09903200	12.07067800	12.01984400
C	30.05547100	12.28051200	10.07266600

H	29.95628000	11.82854600	9.06061300
H	29.77808500	13.35127300	9.95177800
C	31.50528800	12.16272900	10.54313500
H	31.81069500	11.09685900	10.60478200
H	32.20456400	12.67208000	9.85036600
H	31.64436100	12.60906800	11.54991200
H	27.25021200	10.16401100	12.08591800
H	26.21817187	8.74020342	11.28280976

Ni-CFA-1

Zn	-0.65124600	2.94426600	-2.69703800
Cl	-0.90947000	4.54966900	-4.17442700
Zn	-0.21985400	0.30034900	-0.30578900
N	1.21034700	2.38053900	-2.11392000
C	2.43464600	2.81919700	-2.52328300
N	1.40956500	1.40824300	-1.21377900
C	2.83273800	3.80216500	-3.45368700
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90383000	1.20747600	2.76867200
Cl	-2.93117300	1.77532100	4.62704800
N	-1.93755700	2.48281900	1.18352000
C	-2.52180300	3.70875200	1.03041200
N	-1.32710000	2.17417300	0.04396600
C	-3.28518000	4.49134300	1.91599900
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.27390389	-0.35439832	0.35485555
N	1.97095900	0.19374400	1.84154400
C	2.24954500	0.36719000	3.18977700
N	0.66637500	0.40937400	1.65459400
C	3.39349100	0.15258200	3.97729500
C	3.27564500	0.32181500	5.35402000
N	-1.48179400	3.14075000	-0.85419800
C	-2.22726000	4.13298900	-0.28493400
C	-2.68119100	5.37804700	-0.76767600
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69791700	1.17225100	-1.00208400
C	3.38447300	2.05365200	-1.80880100
C	4.76567700	2.21611700	-2.01802100
C	5.17328800	3.18502400	-2.93042800
H	5.49198000	1.57911400	-1.49278100
N	0.07382200	0.77739600	2.79048900
C	1.01308500	0.72854400	3.77010200
C	0.88045700	0.91432400	5.16239200
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48727400	-0.45876500	1.75237300
C	-3.45840900	-1.38129400	2.01243900

N	-1.88973200	-0.80079400	0.61586800
C	-4.39762200	-1.50246300	3.05748500
C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.69840900	-2.72735700	-1.60193400
Cl	-2.64731400	-4.55158100	-2.38475100
N	-1.73404100	-1.02963000	-2.72091800
C	-2.26408500	-0.77699900	-3.95371700
N	-1.21563600	0.10266000	-2.25792300
C	-2.92036800	-1.61552900	-4.87283700
C	-3.35131100	-1.04003100	-6.06579400
N	-2.42151000	-1.90893600	0.11374100
C	-3.41787100	-2.31658700	0.95386900
C	-4.31059400	-3.40170900	0.87963300
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37558400	1.09170300	-3.12972400
C	-2.03120800	0.59171900	-4.21779700
C	-2.46163000	1.18452200	-5.42316200
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27220900	-2.70141400	-1.13973200
C	1.26084400	-3.63229300	-1.23688900
N	0.81955200	-1.57875400	-0.66897500
C	1.24387200	-4.97587000	-1.66665200
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12406400	-1.72655100	-0.46271400
C	2.45740900	-3.01944200	-0.80014000
C	3.68418600	-3.70923000	-0.78633800
C	3.67973400	-5.03713800	-1.20457100
H	4.61464600	-3.21415600	-0.48484800
H	-3.05604700	-2.68397400	-4.64962800
H	4.19922800	-0.53513500	3.73828700
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100

C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700
C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300

N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400
H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	5.05973589	0.39374068	0.79629955
H	5.17246989	1.39709868	0.36128655
H	5.22521089	0.36112968	1.88411555
C	5.23314500	-0.77777200	0.05642100
H	3.57076289	-1.37355232	1.29613455
C	5.69528400	-1.00590100	-1.37490900
H	4.85995200	-1.41335600	-1.98639100
H	5.98283200	-0.06456200	-1.87902600
C	6.87507100	-1.98937200	-1.44543200
H	7.76753900	-1.53380600	-0.96242600
H	6.64367500	-2.89311200	-0.83702800
H	5.46972800	-1.65692100	0.68611700
C	7.21609100	-2.43920900	-2.86827800
H	6.29363400	-2.84388600	-3.34228800
H	7.50419000	-1.55362100	-3.47744000
C	8.32153300	-3.49468200	-2.91642400
H	8.55182900	-3.79991400	-3.95688300
H	9.26194900	-3.11761300	-2.46335900
H	8.02799600	-4.40683000	-2.35571900

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Ni-MFU-4l

Zn	21.26076400	9.80402500	5.92161200
Cl	20.05640800	11.09103200	4.60373400
Zn	23.22342100	7.66666200	8.07546700
N	22.51925400	10.62728900	7.28663900
C	22.85379000	11.90102400	7.61962300
N	23.22593200	9.82010400	8.07413300
C	22.40369900	13.12225900	7.07733900
C	22.94287800	14.27123900	7.62280700
H	21.67153300	13.16986000	6.25880900
Zn	21.03203000	5.57760900	10.02028500
Cl	19.69806700	4.27877300	11.19317300
N	20.24497900	6.91111300	8.69259900

C	18.95637100	7.22547000	8.38026400
N	21.04387900	7.67745600	7.95424300
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66846500	5.92640500	9.61087700
Ni	25.20282600	9.66231200	10.21620800
N	23.90878100	8.34599800	11.01921900
C	23.63123000	8.03843500	12.32611300
N	23.09175300	7.63532800	10.23920100
C	24.16440900	8.47594900	13.55575600
C	23.63167500	7.90624900	14.69382000
N	20.33683200	8.48513700	7.16897200
C	19.01672100	8.24104300	7.39762800
C	17.85133600	8.80037700	6.83529300
C	16.65118000	8.29983100	7.29796700
H	17.88524600	9.58823900	6.06941900
N	24.02769400	10.51668200	8.89610300
C	23.79888200	11.85189100	8.66976500
C	24.33784700	13.02695200	9.22902000
C	23.90450100	14.22035000	8.68927600
H	25.15312200	13.07074500	9.94558100
N	22.30981900	6.83840400	10.96451000
C	22.61203700	7.05895800	12.27055200
C	22.06945000	6.47882000	13.43552400
C	22.59041200	6.91662500	14.63694700
H	21.27649600	5.71819600	13.40071900
N	22.38544000	4.72180000	8.75085800
C	22.66028900	3.41765800	8.46707500
N	23.20233600	5.47952200	8.02446300
C	22.09628400	2.21746600	8.94586100
C	22.62174800	1.04783200	8.43285600
H	21.28289400	2.20201400	9.68522100
Zn	25.37910400	5.60593200	6.05053100
Cl	26.70092700	4.34491600	4.81912500
N	24.12915300	6.93416900	5.14502900
C	23.92462400	7.24378200	3.83402300
N	23.32197600	7.69748500	5.87692600
C	24.50789600	6.74361500	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00548100	4.73011200	7.27333200
C	23.70625600	3.42283000	7.51470300
C	24.24096000	2.22720600	6.99294100
C	23.68565700	1.05498700	7.46445000
H	25.05321200	2.21764100	6.25241900
N	22.59428200	8.49830300	5.10305400
C	22.93495900	8.25376000	3.80676600
C	22.47909500	8.81547600	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71012600	9.60036600	2.56381200
N	26.19174800	6.85890000	7.42892900
C	27.47473000	7.09673700	7.81550000

N	25.39740600	7.61871400	8.18348200
C	28.69606600	6.55975600	7.35869500
C	29.83970100	7.02435300	7.97882700
H	28.74762600	5.81561900	6.55107500
N	26.09265700	8.36614200	9.03509900
C	27.42202800	8.05136700	8.85756100
C	28.58974400	8.50207800	9.50290100
C	29.78335200	7.98755500	9.04356100
H	28.59925200	9.22780200	10.32405200
H	25.27748900	5.95881800	2.65995700
C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53120600	6.08341900	-1.97659900
C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19606000	9.15990300	10.63120900
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700
C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98623600	6.04155300	9.40991700
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00239500	-2.42586600	6.17322900
O	31.04336600	6.52911700	7.55232400
O	30.93535200	8.43359400	9.64540700
H	33.42566700	5.73148100	6.89580600
N	35.89849200	6.62617800	8.09855600
N	35.82007300	8.08910100	9.69179900
N	36.63425300	7.31216200	8.91630900
O	22.09459100	-0.13453800	8.87777700
O	24.18755800	-0.12437300	6.97341000
H	21.24684100	-2.48585700	9.58770800
N	22.25559600	-5.01193000	8.60483600
N	23.85683100	-5.00587300	7.14855900
N	23.01588200	-5.78434000	7.89323800
C	23.63027400	7.76263300	17.05262700

C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27565900	5.46719000	18.08317100
O	22.08336300	6.37260300	15.78728600
O	24.13902600	8.31662300	15.90318200
H	24.96148100	8.95241600	18.25395000
N	23.86366400	7.75796200	20.76033000
N	22.29153800	6.27316000	20.66859100
N	23.04539800	6.93878300	21.48671900
H	24.95942900	9.22592400	13.63887000
O	22.63029500	8.84979700	0.24880300
O	24.60929500	6.82783000	0.30316700
H	21.98416500	9.71176700	-2.11545900
N	24.61766600	7.23706900	-4.57554900
N	23.87394900	8.06355800	-5.37016100
N	23.10407500	8.78372300	-4.61530200
O	15.37922200	6.79369300	8.73226700
H	13.24527300	9.68618100	5.88613200
O	15.50009300	8.82606800	6.76711700
N	10.60807100	8.65157200	6.83227900
N	10.51713500	7.09722100	8.33575700
N	9.78609900	7.85868700	7.58281100
C	23.05992300	16.63156900	7.64155300
C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30580000	17.64300000	10.05255800
O	22.53380400	15.47493300	7.11131500
O	24.44705900	15.37641600	9.19876300
H	21.89075000	17.85631200	6.30362500
N	22.94640400	20.33775300	7.34835900
N	23.68170000	21.07828000	8.11759400
N	24.40335100	20.26652300	8.94733100
H	24.52893600	8.36031600	21.24648300
H	10.19956600	9.31895900	6.17681300
H	24.53054200	-5.45085500	6.52406900
H	36.23397200	8.69936500	10.39760000
H	25.04007500	20.68394100	9.62711800
H	25.28396000	6.59430100	-5.00544100
C	24.91011000	10.95140500	11.60402400
H	24.62459000	11.95724100	11.27018400
C	26.36136100	10.67898400	11.77513400
H	26.64664400	9.75173700	11.08319200
H	24.21487300	10.59322400	12.37841100
C	27.35051100	11.80732700	11.45011600
H	28.38062600	11.39264300	11.40354800

H	27.13674500	12.19009900	10.42968700
C	27.29972100	12.94537000	12.47050500
H	27.52662900	12.57968000	13.49352000
H	28.03438700	13.73821100	12.22652800
H	26.29449300	13.41388700	12.50324200
H	26.60416700	10.21280200	12.75717300

Ni-CFA-1

Zn	-0.64791400	2.94407900	-2.69670700
Cl	-0.90945800	4.54962900	-4.17446000
Zn	-0.21556900	0.29903300	-0.30406600
N	1.21047600	2.38084800	-2.11363600
C	2.43474100	2.81927000	-2.52334600
N	1.40870700	1.40869000	-1.21319000
C	2.83273800	3.80211500	-3.45374100
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90255200	1.20834100	2.76836100
Cl	-2.93116900	1.77531900	4.62705100
N	-1.93758000	2.48277600	1.18352200
C	-2.52182200	3.70874200	1.03040200
N	-1.32704800	2.17424500	0.04392900
C	-3.28517200	4.49134700	1.91600200
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.18670600	-0.21097000	0.29462600
N	1.96676300	0.14525600	1.85434100
C	2.24954700	0.36736900	3.19061300
N	0.66645000	0.41006900	1.65507300
C	3.39346000	0.15235400	3.97727700
C	3.27563800	0.32178700	5.35402300
N	-1.48168800	3.14071500	-0.85425300
C	-2.22728900	4.13297600	-0.28494900
C	-2.68118200	5.37805200	-0.76767200
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69546000	1.16415900	-1.02476800
C	3.38388200	2.05261500	-1.80895700
C	4.76565700	2.21574700	-2.01843900
C	5.17329100	3.18508600	-2.93036200
H	5.49198900	1.57929900	-1.49257200
N	0.07381900	0.77758300	2.79042000
C	1.01306700	0.72862500	3.77003200
C	0.88043800	0.91423500	5.16240200
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48727800	-0.45881000	1.75238100
C	-3.45840000	-1.38130100	2.01245200
N	-1.88972000	-0.80072400	0.61587200
C	-4.39762700	-1.50245800	3.05748000

C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.69845200	-2.72659500	-1.60191300
Cl	-2.64734400	-4.55161000	-2.38468100
N	-1.73400600	-1.02969300	-2.72089400
C	-2.26407100	-0.77700800	-3.95372400
N	-1.21564700	0.10260400	-2.25788900
C	-2.92036500	-1.61553000	-4.87283900
C	-3.35131100	-1.04003100	-6.06579400
N	-2.42157800	-1.90889300	0.11376900
C	-3.41785500	-2.31659600	0.95388500
C	-4.31060100	-3.40170200	0.87962700
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37563900	1.09163500	-3.12976500
C	-2.03120900	0.59171900	-4.21779600
C	-2.46163500	1.18452300	-5.42315900
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27220800	-2.70114100	-1.14033100
C	1.26080800	-3.63203800	-1.23713200
N	0.82033500	-1.57879800	-0.66984600
C	1.24383600	-4.97592700	-1.66647000
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12700900	-1.71816800	-0.45743200
C	2.45791800	-3.02004800	-0.80044500
C	3.68413400	-3.70931600	-0.78599400
C	3.67973400	-5.03714000	-1.20456600
H	4.61466600	-3.21412300	-0.48496600
H	-3.05604700	-2.68397400	-4.64962800
H	4.19925300	-0.53509700	3.73826200
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100

H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700
C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400

N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400
H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	4.60858700	0.82150800	1.05151700
H	4.98521000	1.62697700	0.40051700
H	4.37591100	1.20251000	2.05963200
C	5.31453800	-0.49035700	0.96803300
H	4.56815900	-1.28030800	0.50842300
C	6.59260600	-0.55266600	0.11536400
H	6.35883500	-0.22490400	-0.91963600
H	7.30188600	0.19861800	0.52397400
C	7.26259300	-1.92523500	0.08642800
H	7.49461500	-2.28369100	1.11100200
H	6.62568200	-2.69290900	-0.39896600
H	5.49400100	-0.93458600	1.97108800
H	8.21533800	-1.89435400	-0.47760300

TS-βH^B

Ni-MFU-4l

Zn	21.25988200	9.80251500	5.92060800
Cl	20.05640800	11.09103200	4.60373400
Zn	23.22120400	7.66521100	8.07681900
N	22.51925400	10.62728900	7.28663900
C	22.85379000	11.90102400	7.61962300
N	23.22593200	9.82010400	8.07413300
C	22.40369900	13.12225900	7.07733900
C	22.94287800	14.27123900	7.62280700
H	21.67153300	13.16986000	6.25880900
Zn	21.03270400	5.57746700	10.02122800
Cl	19.69806700	4.27877300	11.19317300
N	20.24497900	6.91111300	8.69259900
C	18.95637100	7.22547000	8.38026400
N	21.04387900	7.67745600	7.95424300
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66846500	5.92640500	9.61087700
Ni	25.28240800	9.64019000	10.28207300
N	23.89382700	8.36301900	11.01603700
C	23.63123000	8.03843500	12.32611300

N	23.09175300	7.63532800	10.23920100
C	24.16440900	8.47594900	13.55575600
C	23.63167500	7.90624900	14.69382000
N	20.33683200	8.48513700	7.16897200
C	19.01672100	8.24104300	7.39762800
C	17.85133600	8.80037700	6.83529300
C	16.65118000	8.29983100	7.29796700
H	17.88524600	9.58823900	6.06941900
N	24.01621000	10.51146000	8.91171600
C	23.79888200	11.85189100	8.66976500
C	24.33784700	13.02695200	9.22902000
C	23.90450100	14.22035000	8.68927600
H	25.15312200	13.07074500	9.94558100
N	22.30981900	6.83840400	10.96451000
C	22.61203700	7.05895800	12.27055200
C	22.06945000	6.47882000	13.43552400
C	22.59041200	6.91662500	14.63694700
H	21.27649600	5.71819600	13.40071900
N	22.38544000	4.72180000	8.75085800
C	22.66028900	3.41765800	8.46707500
N	23.20233600	5.47952200	8.02446300
C	22.09628400	2.21746600	8.94586100
C	22.62174800	1.04783200	8.43285600
H	21.28289400	2.20201400	9.68522100
Zn	25.37843800	5.60510900	6.05014100
Cl	26.70092700	4.34491600	4.81912500
N	24.12915300	6.93416900	5.14502900
C	23.92462400	7.24378200	3.83402300
N	23.32197600	7.69748500	5.87692600
C	24.50789600	6.74361500	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00548100	4.73011200	7.27333200
C	23.70625600	3.42283000	7.51470300
C	24.24096000	2.22720600	6.99294100
C	23.68565700	1.05498700	7.46445000
H	25.05321200	2.21764100	6.25241900
N	22.59428200	8.49830300	5.10305400
C	22.93495900	8.25376000	3.80676600
C	22.47909500	8.81547600	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71012600	9.60036600	2.56381200
N	26.19174800	6.85890000	7.42892900
C	27.47473000	7.09673700	7.81550000
N	25.39740600	7.61871400	8.18348200
C	28.69606600	6.55975600	7.35869500
C	29.83970100	7.02435300	7.97882700
H	28.74762600	5.81561900	6.55107500
N	26.09730900	8.36361600	9.03428800
C	27.42202800	8.05136700	8.85756100
C	28.58974400	8.50207800	9.50290100
C	29.78335200	7.98755500	9.04356100

H	28.59925200	9.22780200	10.32405200
H	25.27748900	5.95881800	2.65995700
C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53120600	6.08341900	-1.97659900
C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19606000	9.15990300	10.63120900
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700
C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98623600	6.04155300	9.40991700
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00239500	-2.42586600	6.17322900
O	31.04336600	6.52911700	7.55232400
O	30.93535200	8.43359400	9.64540700
H	33.42566700	5.73148100	6.89580600
N	35.89849200	6.62617800	8.09855600
N	35.82007300	8.08910100	9.69179900
N	36.63425300	7.31216200	8.91630900
O	22.09459100	-0.13453800	8.87777700
O	24.18755800	-0.12437300	6.97341000
H	21.24684100	-2.48585700	9.58770800
N	22.25559600	-5.01193000	8.60483600
N	23.85683100	-5.00587300	7.14855900
N	23.01588200	-5.78434000	7.89323800
C	23.63027400	7.76263300	17.05262700
C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27565900	5.46719000	18.08317100
O	22.08336300	6.37260300	15.78728600
O	24.13902600	8.31662300	15.90318200

H	24.96148100	8.95241600	18.25395000
N	23.86366400	7.75796200	20.76033000
N	22.29153800	6.27316000	20.66859100
N	23.04539800	6.93878300	21.48671900
H	24.95942900	9.22592400	13.63887000
O	22.63029500	8.84979700	0.24880300
O	24.60929500	6.82783000	0.30316700
H	21.98416500	9.71176700	-2.11545900
N	24.61766600	7.23706900	-4.57554900
N	23.87394900	8.06355800	-5.37016100
N	23.10407500	8.78372300	-4.61530200
O	15.37922200	6.79369300	8.73226700
H	13.24527300	9.68618100	5.88613200
O	15.50009300	8.82606800	6.76711700
N	10.60807100	8.65157200	6.83227900
N	10.51713500	7.09722100	8.33575700
N	9.78609900	7.85868700	7.58281100
C	23.05992300	16.63156900	7.64155300
C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30580000	17.64300000	10.05255800
O	22.53380400	15.47493300	7.11131500
O	24.44705900	15.37641600	9.19876300
H	21.89075000	17.85631200	6.30362500
N	22.94640400	20.33775300	7.34835900
N	23.68170000	21.07828000	8.11759400
N	24.40335100	20.26652300	8.94733100
H	24.52893600	8.36031600	21.24648300
H	10.19956600	9.31895900	6.17681300
H	24.53054200	-5.45085500	6.52406900
H	36.23397200	8.69936500	10.39760000
H	25.04007500	20.68394100	9.62711800
H	25.28396000	6.59430100	-5.00544100
C	25.11924900	11.07540700	11.60323100
H	24.52417500	11.90408300	11.20628000
C	26.51926100	10.90865600	11.29675900
H	26.42371800	9.32616300	11.12526900
H	24.75215100	10.72739900	12.57802700
C	27.33591800	11.81567400	10.38405700
H	28.26857800	11.28923400	10.09550500
H	26.80483600	11.99981500	9.42960800
C	27.69726900	13.14412100	11.06381500
H	28.24103200	12.97460600	12.01601800
H	28.34249000	13.76525300	10.41050700
H	26.79167900	13.73878200	11.30620400
H	27.13145800	10.56578400	12.15916300

Ni-CFA-1

Zn	-0.65098500	2.94386100	-2.69676600
Cl	-0.90945800	4.54962900	-4.17446000
Zn	-0.21794200	0.29985200	-0.30072100
N	1.21047600	2.38084800	-2.11363600
C	2.43474100	2.81927000	-2.52334600
N	1.40870700	1.40869000	-1.21319000
C	2.83273800	3.80211500	-3.45374100
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400
Zn	-1.90061800	1.20746700	2.76991700
Cl	-2.93116900	1.77531900	4.62705100
N	-1.93758000	2.48277600	1.18352200
C	-2.52182200	3.70874200	1.03040200
N	-1.32704800	2.17424500	0.04392900
C	-3.28517200	4.49134700	1.91600200
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.27139300	-0.30320100	0.30470200
N	1.96732300	0.17313200	1.84520000
C	2.24954700	0.36736900	3.19061300
N	0.66645000	0.41006900	1.65507300
C	3.39346000	0.15235400	3.97727700
C	3.27563800	0.32178700	5.35402300
N	-1.48168800	3.14071500	-0.85425300
C	-2.22728900	4.13297600	-0.28494900
C	-2.68118200	5.37805200	-0.76767200
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69467400	1.17138600	-1.00547500
C	3.38388200	2.05261500	-1.80895700
C	4.76565700	2.21574700	-2.01843900
C	5.17329100	3.18508600	-2.93036200
H	5.49198900	1.57929900	-1.49257200
N	0.07381900	0.77758300	2.79042000
C	1.01306700	0.72862500	3.77003200
C	0.88043800	0.91423500	5.16240200
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48727800	-0.45881000	1.75238100
C	-3.45840000	-1.38130100	2.01245200
N	-1.88972000	-0.80072400	0.61587200
C	-4.39762700	-1.50245800	3.05748000
C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.69949200	-2.72664800	-1.60153800
Cl	-2.64734400	-4.55161000	-2.38468100
N	-1.73400600	-1.02969300	-2.72089400
C	-2.26407100	-0.77700800	-3.95372400
N	-1.21564700	0.10260400	-2.25788900
C	-2.92036500	-1.61553000	-4.87283900

C	-3.35131100	-1.04003100	-6.06579400
N	-2.42157800	-1.90889300	0.11376900
C	-3.41785500	-2.31659600	0.95388500
C	-4.31060100	-3.40170200	0.87962700
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37563900	1.09163500	-3.12976500
C	-2.03120900	0.59171900	-4.21779600
C	-2.46163500	1.18452300	-5.42315900
C	-3.11302500	0.35561900	-6.31704800
H	-2.28929500	2.25276300	-5.62020300
N	0.27220800	-2.70114100	-1.14033100
C	1.26080800	-3.63203800	-1.23713200
N	0.82033500	-1.57879800	-0.66984600
C	1.24383600	-4.97592700	-1.66647000
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12961700	-1.72164100	-0.46983800
C	2.45791800	-3.02004800	-0.80044500
C	3.68413400	-3.70931600	-0.78599400
C	3.67973400	-5.03714000	-1.20456600
H	4.61466600	-3.21412300	-0.48496600
H	-3.05604700	-2.68397400	-4.64962800
H	4.19925300	-0.53509700	3.73826200
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700

C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300
H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400

H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	4.83576600	0.69274000	0.95997300
H	4.99229100	1.59345500	0.35190500
H	4.75375900	0.89308100	2.03931700
C	5.30279500	-0.59174300	0.52927000
H	3.88939500	-1.39973000	1.01309900
C	6.06413500	-0.86164900	-0.75953300
H	6.03987500	-1.94955800	-0.97644200
H	5.56678500	-0.38143400	-1.62513100
C	7.52854000	-0.40862300	-0.66012500
H	7.60886500	0.68612600	-0.50231100
H	8.04584000	-0.90154800	0.18833300
H	5.65625100	-1.25013200	1.34991700
H	8.08580600	-0.65531900	-1.58586900

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Ni-MFU-4l

Zn	21.25898700	9.80153900	5.91943800
Cl	20.05642000	11.09103200	4.60372400
Zn	23.22197100	7.66358900	8.07049500
N	22.51922700	10.62731200	7.28668100
C	22.85378800	11.90106100	7.61962700
N	23.22586400	9.81998100	8.07420600
C	22.40372100	13.12225800	7.07731900
C	22.94287800	14.27123900	7.62280700
H	21.67153300	13.16986000	6.25880900
Zn	21.03106000	5.57525800	10.01807200
Cl	19.69806600	4.27877100	11.19317000
N	20.24497500	6.91111300	8.69259700
C	18.95637100	7.22547100	8.38026500
N	21.04387300	7.67745900	7.95423600
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66846500	5.92640500	9.61087700
Ni	25.29419400	9.59605400	10.33232500
N	23.88097100	8.37600700	11.01656300
C	23.63121600	8.03851200	12.32609800
N	23.09182000	7.63535800	10.23915700
C	24.16439200	8.47593100	13.55577000
C	23.63168800	7.90623600	14.69381900
N	20.33683400	8.48514500	7.16897200
C	19.01672000	8.24104500	7.39762600
C	17.85133600	8.80037800	6.83529400
C	16.65118000	8.29983100	7.29796700
H	17.88524600	9.58823900	6.06941900
N	24.01641300	10.51056400	8.91646800

C	23.79888800	11.85175700	8.66977200
C	24.33785500	13.02695900	9.22899800
C	23.90450900	14.22035000	8.68926900
H	25.15311500	13.07074400	9.94558900
N	22.30982100	6.83840700	10.96451800
C	22.61203300	7.05896200	12.27056100
C	22.06946200	6.47880700	13.43552300
C	22.59041200	6.91662500	14.63694700
H	21.27649600	5.71819600	13.40071900
N	22.38544200	4.72180400	8.75086100
C	22.66029000	3.41765800	8.46707500
N	23.20231900	5.47952000	8.02446900
C	22.09628300	2.21746600	8.94586000
C	22.62174800	1.04783200	8.43285600
H	21.28289400	2.20201400	9.68522100
Zn	25.38043200	5.60593200	6.05053800
Cl	26.70092800	4.34490900	4.81913000
N	24.12915800	6.93416100	5.14504200
C	23.92462200	7.24378100	3.83402300
N	23.32198000	7.69747800	5.87692600
C	24.50789700	6.74361600	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00547200	4.73009600	7.27333400
C	23.70625800	3.42283000	7.51470500
C	24.24095900	2.22720600	6.99294000
C	23.68565700	1.05498700	7.46445000
H	25.05321200	2.21764100	6.25241900
N	22.59428500	8.49829500	5.10305300
C	22.93496000	8.25375600	3.80676700
C	22.47909500	8.81547600	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71012600	9.60036600	2.56381200
N	26.19174100	6.85894000	7.42888600
C	27.47471600	7.09673900	7.81550000
N	25.39742900	7.61892800	8.18337000
C	28.69606600	6.55975500	7.35869600
C	29.83970100	7.02435300	7.97882700
H	28.74762600	5.81561900	6.55107500
N	26.09853600	8.35078100	9.03792000
C	27.42203500	8.05127500	8.85764300
C	28.58973300	8.50203900	9.50294800
C	29.78335400	7.98757100	9.04354700
H	28.59925400	9.22782600	10.32403100
H	25.27748900	5.95881800	2.65995700
C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53120600	6.08341900	-1.97659900

C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19606000	9.15990300	10.63120900
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700
C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98623600	6.04155300	9.40991700
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00239500	-2.42586600	6.17322900
O	31.04336600	6.52911700	7.55232400
O	30.93535200	8.43359400	9.64540700
H	33.42566700	5.73148100	6.89580600
N	35.89849200	6.62617800	8.09855600
N	35.82007300	8.08910100	9.69179900
N	36.63425300	7.31216200	8.91630900
O	22.09459100	-0.13453800	8.87777700
O	24.18755800	-0.12437300	6.97341000
H	21.24684100	-2.48585700	9.58770800
N	22.25559600	-5.01193000	8.60483600
N	23.85683100	-5.00587300	7.14855900
N	23.01588200	-5.78434000	7.89323800
C	23.63027400	7.76263300	17.05262700
C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27565900	5.46719000	18.08317100
O	22.08336300	6.37260300	15.78728600
O	24.13902600	8.31662300	15.90318200
H	24.96148100	8.95241600	18.25395000
N	23.86366400	7.75796200	20.76033000
N	22.29153800	6.27316000	20.66859100
N	23.04539800	6.93878300	21.48671900
H	24.95943300	9.22591900	13.63887000
O	22.63029500	8.84979700	0.24880300
O	24.60929500	6.82783000	0.30316700
H	21.98416500	9.71176700	-2.11545900
N	24.61766600	7.23706900	-4.57554900

N	23.87394900	8.06355800	-5.37016100
N	23.10407500	8.78372300	-4.61530200
O	15.37922200	6.79369300	8.73226700
H	13.24527300	9.68618100	5.88613200
O	15.50009300	8.82606800	6.76711700
N	10.60807100	8.65157200	6.83227900
N	10.51713500	7.09722100	8.33575700
N	9.78609900	7.85868700	7.58281100
C	23.05992300	16.63156900	7.64155300
C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30580000	17.64300000	10.05255800
O	22.53380400	15.47493300	7.11131500
O	24.44705900	15.37641600	9.19876300
H	21.89075000	17.85631200	6.30362500
N	22.94640400	20.33775300	7.34835900
N	23.68170000	21.07828000	8.11759400
N	24.40335100	20.26652300	8.94733100
H	24.52893600	8.36031600	21.24648300
H	10.19956600	9.31895900	6.17681300
H	24.53054200	-5.45085500	6.52406900
H	36.23397200	8.69936500	10.39760000
H	25.04007500	20.68394100	9.62711800
H	25.28396000	6.59430100	-5.00544100
C	25.52433353	11.15582342	11.49470078
H	24.71915553	11.87144442	11.28382078
C	26.67306100	10.99602800	10.72420200
H	26.10290200	8.92791100	11.28869700
H	25.59249353	10.88509642	12.55980078
C	27.20634700	11.75169100	9.52047700
H	27.96920400	11.10635600	9.03713000
H	26.43524400	11.90933000	8.74456300
C	27.86116400	13.08935600	9.90076600
H	28.65164700	12.94689700	10.66609300
H	28.32720000	13.56975600	9.01683600
H	27.12403900	13.80541000	10.32056400
H	27.50645700	10.56367200	11.31126100

Ni-CFA-1

Zn	-0.65164000	2.94426300	-2.69709800
Cl	-0.90945800	4.54963700	-4.17445500
Zn	-0.22109200	0.29971400	-0.30556600
N	1.21042900	2.38083300	-2.11363500
C	2.43473000	2.81924700	-2.52335200
N	1.40883800	1.40866300	-1.21326600
C	2.83273800	3.80213400	-3.45372100
C	4.19307400	3.96721700	-3.63138900
H	2.08675000	4.40340400	-3.99425400

Zn	-1.90421300	1.20753000	2.76860500
Cl	-2.93117100	1.77531000	4.62705100
N	-1.93757700	2.48279500	1.18352000
C	-2.52182700	3.70873900	1.03040000
N	-1.32704800	2.17424500	0.04391800
C	-3.28517200	4.49134700	1.91600200
C	-3.74061400	5.72219600	1.44896000
H	-3.52247400	4.11517400	2.92205900
Ni	3.26680000	-0.34026400	0.36467900
N	1.97129000	0.19047900	1.84202000
C	2.24945600	0.36717000	3.19063700
N	0.66641600	0.40993700	1.65513300
C	3.39350000	0.15243800	3.97724200
C	3.27564100	0.32179900	5.35402200
N	-1.48169600	3.14071200	-0.85425300
C	-2.22729000	4.13297400	-0.28494700
C	-2.68118300	5.37805200	-0.76767200
C	-3.42380000	6.14357800	0.11109900
H	-2.43777600	5.71196700	-1.78692300
N	2.69590600	1.17135300	-1.00226900
C	3.38390700	2.05254800	-1.80909800
C	4.76566100	2.21578600	-2.01838300
C	5.17329100	3.18509400	-2.93035300
H	5.49198800	1.57928900	-1.49258400
N	0.07383300	0.77762300	2.79041300
C	1.01308300	0.72868500	3.77002700
C	0.88044100	0.91424700	5.16240100
C	2.01670400	0.71101400	5.92355500
H	-0.09436000	1.16379100	5.60669200
N	-2.48727700	-0.45879600	1.75237500
C	-3.45839800	-1.38130200	2.01245400
N	-1.88971800	-0.80072600	0.61585800
C	-4.39762600	-1.50245900	3.05748100
C	-5.26727600	-2.57364300	2.97938200
H	-4.41867500	-0.77915700	3.88583600
Zn	-1.69832700	-2.72757200	-1.60197900
Cl	-2.64734600	-4.55160800	-2.38467900
N	-1.73401400	-1.02968400	-2.72091300
C	-2.26407000	-0.77700900	-3.95372400
N	-1.21565300	0.10261400	-2.25789700
C	-2.92036600	-1.61553000	-4.87283800
C	-3.35131100	-1.04003100	-6.06579400
N	-2.42156300	-1.90888700	0.11375000
C	-3.41785500	-2.31659500	0.95388600
C	-4.31060000	-3.40170300	0.87962700
C	-5.24634900	-3.52764300	1.90386500
H	-4.27255500	-4.09313100	0.02498000
N	-1.37562700	1.09163800	-3.12977200
C	-2.03120400	0.59172000	-4.21780000
C	-2.46163600	1.18452300	-5.42315900
C	-3.11302500	0.35561900	-6.31704800

H	-2.28929500	2.25276300	-5.62020300
N	0.27224700	-2.70117400	-1.14031300
C	1.26083000	-3.63205200	-1.23717100
N	0.82019900	-1.57878600	-0.66953400
C	1.24383400	-4.97593000	-1.66646200
C	2.45122300	-5.64763000	-1.63522300
H	0.30832100	-5.45260300	-1.99407400
N	2.12338000	-1.72809800	-0.46217300
C	2.45797400	-3.01979900	-0.80057500
C	3.68411300	-3.70935300	-0.78602000
C	3.67973000	-5.03714600	-1.20454700
H	4.61466300	-3.21412800	-0.48495000
H	-3.05604700	-2.68397400	-4.64962800
H	4.19924100	-0.53511600	3.73827500
C	-4.55753300	6.60324200	2.32699100
C	-4.28036000	6.66307500	3.72747500
C	-5.60272600	7.36577000	1.80015000
C	-5.00953200	7.44938000	4.60740100
H	-3.44034300	6.07059300	4.11937500
C	-6.35173900	8.16691200	2.67527200
H	-5.86575600	7.33190000	0.73362100
C	-6.05734700	8.20420400	4.05616700
H	-4.76498000	7.47812200	5.67878300
H	-7.14521600	9.39652900	5.50373300
C	6.62360000	3.41003400	-3.17581500
C	7.09323300	3.68537300	-4.49598700
C	7.53724700	3.34114600	-2.12074400
C	8.43357600	3.89011100	-4.79226100
H	6.36049800	3.71157900	-5.31623300
C	8.89642900	3.54628200	-2.40088000
H	7.21143600	3.16112400	-1.08661100
C	9.33305600	3.81748700	-3.71687800
H	8.76405500	4.08987000	-5.82158100
H	11.40231400	4.15782000	-4.26934200
C	4.45735800	0.08323500	6.22565700
C	4.73876100	0.95679200	7.31890200
C	5.84813400	0.80098700	8.13890400
H	4.05769400	1.80169800	7.50019300
C	5.31371500	-0.98730500	5.96017400
C	6.70232500	-0.27444300	7.84545200
H	6.04410700	1.49671800	8.96718700
C	6.44294800	-1.15739500	6.77383300
H	5.11774400	-1.70663200	5.15206400
C	-6.22853200	-4.64529300	1.88611500
C	-5.82759600	-5.93351500	1.41558100
C	-6.70053700	-7.00803900	1.36208400
H	-4.78187200	-6.07243100	1.10455000
C	-7.54342900	-4.43481500	2.31615600
C	-8.02243500	-6.79773700	1.79123500
H	-6.38142400	-7.99759500	1.00596500
C	-8.42151100	-5.52557300	2.25891300

H	-7.87612500	-3.44302100	2.65408300
H	-10.42657200	-5.05391000	2.93925100
C	-4.06277800	-1.86687000	-7.07787100
C	-3.83039900	-1.65181200	-8.47087600
C	-4.45658900	-2.40357400	-9.45246400
H	-3.10699600	-0.87810200	-8.76706900
C	-4.95082300	-2.86527300	-6.66193600
C	-5.34888400	-3.40643400	-9.03639800
H	-4.26443000	-2.23823600	-10.52189300
C	-5.57890500	-3.62277400	-7.65902400
H	-5.15662300	-3.02847100	-5.59445800
H	-6.92379900	-5.13073200	-6.87179000
C	4.94319900	-5.82300300	-1.21018900
C	5.90386300	-5.62434500	-0.17104600
C	7.10321000	-6.31594900	-0.12516500
H	5.65646200	-4.92425500	0.64015100
C	5.19843300	-6.74575800	-2.23054200
C	7.36152600	-7.24207200	-1.15053000
H	7.82811300	-6.17303400	0.68712900
C	6.41364600	-7.44241900	-2.17915200
H	4.48343900	-6.89133800	-3.05265300
H	6.68216200	-8.82794200	-3.82636400
N	8.44938500	-8.06614200	-1.37868100
N	8.23376800	-8.74373600	-2.46225300
N	7.01530100	-8.38752600	-2.96798400
N	-6.48592300	-4.64991100	-7.65857700
N	-6.78556200	-5.03839300	-8.93292500
N	-6.11407900	-4.30219400	-9.76247700
N	11.05780700	3.78205400	-2.26581800
N	9.99837800	3.53977000	-1.56028000
N	10.68776200	3.95468400	-3.56946300
N	-7.42945200	9.00270700	2.42856300
N	-7.80099800	9.53926000	3.54747400
N	-6.99151500	9.07648200	4.54691000
N	-9.10673100	-7.65550300	1.85159000
N	-10.12568800	-7.00160200	2.31465600
N	-9.74332000	-5.71466500	2.56757400
N	7.44552000	-2.11276900	6.73161300
N	8.28557700	-1.87124200	7.68818500
N	7.86305200	-0.77038800	8.37728600
H	8.41141500	-0.43703500	9.17107400
H	-5.99866300	-2.72322600	3.78737900
H	4.54875800	4.74209000	-4.32667000
H	2.47788200	-6.70710900	-1.93008200
H	1.94755500	0.81433500	7.01742000
H	-3.48957900	0.78250000	-7.25823400
H	-3.77493700	7.13392200	-0.21431400
C	5.04045311	0.40177403	0.75084512
H	5.08556411	1.42854703	0.35997712
H	5.27720811	0.32715803	1.82356212
C	5.20833900	-0.72562300	-0.04190000

H	3.60272900	-1.35809900	1.29619200
C	5.59480200	-0.84999700	-1.50513500
H	5.36814900	-1.88430200	-1.83487100
H	4.97748800	-0.20589100	-2.15786000
C	7.08968500	-0.57709800	-1.73846000
H	7.36667400	0.46486100	-1.47648800
H	7.72055000	-1.24746600	-1.11984100
H	5.54591300	-1.60904200	0.53483800
H	7.36203600	-0.73845000	-2.80093100

β_{HC}

Ni-MFU-4l

Zn	21.26627400	9.80469700	5.92836200
Cl	20.06115500	11.08522100	4.61110200
Zn	23.22131600	7.67498700	8.07575900
N	22.52048600	10.62622800	7.28760300
C	22.85376600	11.90100900	7.61964400
N	23.22573900	9.81896800	8.07640600
C	22.40372000	13.12225800	7.07732000
C	22.94287800	14.27123900	7.62280700
H	21.67161600	13.17040700	6.25908000
Zn	21.03472300	5.57985000	10.01473400
Cl	19.70540100	4.28471900	11.18919300
N	20.24544600	6.91181700	8.69342000
C	18.95637100	7.22546800	8.38026200
N	21.04500000	7.67823900	7.95619500
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66781400	5.92669900	9.61077100
Ni	25.31014900	9.53634200	10.41761400
N	23.90631700	8.36072600	11.02470100
C	23.63096600	8.03858500	12.32621500
N	23.09216200	7.63717000	10.23835900
C	24.16435500	8.47601200	13.55575700
C	23.63164500	7.90628000	14.69382200
N	20.33772800	8.48535400	7.17067200
C	19.01672100	8.24104400	7.39762900
C	17.85133600	8.80037700	6.83529300
C	16.65118000	8.29983100	7.29796700
H	17.88463200	9.58818200	6.06967500
N	24.01581000	10.51124300	8.90733500
C	23.79902400	11.85165800	8.66986500
C	24.33790500	13.02694700	9.22897400
C	23.90452200	14.22034900	8.68925700
H	25.15352000	13.06988600	9.94547500
N	22.31104200	6.83942600	10.96321600
C	22.61198100	7.05901800	12.27056800
C	22.06943300	6.47883700	13.43552500
C	22.59041200	6.91662500	14.63694700
H	21.27660600	5.71839200	13.40136300

N	22.38615200	4.72237100	8.75127100
C	22.66029100	3.41765800	8.46707600
N	23.20358700	5.48070500	8.02624300
C	22.09628400	2.21746600	8.94586100
C	22.62174800	1.04783200	8.43285600
H	21.28320700	2.20140000	9.68518900
Zn	25.37348600	5.60959700	6.05252200
Cl	26.69495200	4.35084200	4.82546500
N	24.12770300	6.93361700	5.14586700
C	23.92462400	7.24378200	3.83402300
N	23.32036800	7.69616400	5.87819600
C	24.50789600	6.74361500	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00626700	4.73091100	7.27520600
C	23.70625700	3.42283000	7.51470400
C	24.24096000	2.22720600	6.99294100
C	23.68565700	1.05498700	7.46445000
H	25.05315300	2.21699300	6.25272100
N	22.59351000	8.49713800	5.10389000
C	22.93495800	8.25376100	3.80676600
C	22.47909500	8.81547600	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71025800	9.60011900	2.56309700
N	26.19068400	6.86247200	7.42761400
C	27.47474200	7.09682200	7.81542300
N	25.39659000	7.62198400	8.18230700
C	28.69606700	6.55976600	7.35868600
C	29.83970100	7.02435300	7.97882700
H	28.74830500	5.81601700	6.55109100
N	26.09240100	8.33492600	9.06412900
C	27.42223100	8.05140800	8.85739200
C	28.58974800	8.50206200	9.50290400
C	29.78335200	7.98755900	9.04355700
H	28.59846800	9.22819800	10.32364200
H	25.27725400	5.95892000	2.65934000
C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53109700	6.08357600	-1.97703600
C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19650900	9.15985000	10.63101000
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700

C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98579600	6.04170800	9.40977800
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00225500	-2.42630400	6.17336600
O	31.04330900	6.52965100	7.55274100
O	30.93540500	8.43361100	9.64449300
H	33.42610700	5.73163600	6.89594100
N	35.89879200	6.62663400	8.09905900
N	35.81985500	8.08939700	9.69222100
N	36.63482700	7.31287100	8.91678600
O	22.09512300	-0.13452700	8.87738200
O	24.18709100	-0.12435500	6.97387300
H	21.24697700	-2.48629900	9.58757400
N	22.25604700	-5.01225200	8.60433500
N	23.85722600	-5.00567800	7.14822100
N	23.01652300	-5.78493100	7.89273700
C	23.63027400	7.76263300	17.05262700
C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27575600	5.46733300	18.08364000
O	22.08380100	6.37312100	15.78725300
O	24.13837300	8.31631900	15.90315500
H	24.96131000	8.95228300	18.25436600
N	23.86404000	7.75833100	20.76015500
N	22.29189200	6.27373500	20.66894800
N	23.04621400	6.93905400	21.48732400
H	24.95825200	9.22703200	13.63857400
O	22.63075600	8.84933200	0.24881600
O	24.60882400	6.82827900	0.30315900
H	21.98432500	9.71164600	-2.11589600
N	24.61804400	7.23671700	-4.57534600
N	23.87445100	8.06289900	-5.37075100
N	23.10459100	8.78328000	-4.61561200
O	15.37926900	6.79418800	8.73182300
H	13.24482700	9.68605100	5.88625200
O	15.50010000	8.82560500	6.76759400
N	10.60828600	8.65194800	6.83193300
N	10.51683800	7.09773400	8.33530400
N	9.78554300	7.85924100	7.58218600
C	23.05992300	16.63156900	7.64155300

C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30567400	17.64348800	10.05242900
O	22.53411200	15.47487300	7.11194800
O	24.44650600	15.37643000	9.19824500
H	21.89098500	17.85675200	6.30368700
N	22.94733900	20.33803400	7.34842300
N	23.68143600	21.07888000	8.11895200
N	24.40377400	20.26630700	8.94763700
H	24.52931700	8.36069900	21.24579500
H	10.20029100	9.31932200	6.17649800
H	24.53094600	-5.45014700	6.52375700
H	36.23323100	8.69958400	10.39805900
H	25.04051300	20.68321200	9.62737600
H	25.28432300	6.59395800	-5.00472000
C	25.27587200	11.10395800	11.60079300
H	24.62211100	11.73061800	10.98599200
C	26.69814200	10.98027500	11.16429800
H	26.86082800	9.88944000	10.70918100
C	27.36752300	11.95414400	10.18717200
H	28.42104900	11.66111700	10.00507800
H	26.86033700	11.97913400	9.20524800
H	27.34043100	10.83684500	12.06144800
H	27.37786800	12.98229500	10.60440000
C	25.00580800	11.41637100	13.05487900
H	23.96542300	11.18674600	13.35648800
H	25.70340300	10.91800800	13.75910300
H	25.14342500	12.51188800	13.20983700

Ni-CFA-1

Zn	-0.91734700	3.34514700	-2.32478100
Cl	-1.06731900	5.02562000	-3.70727800
Zn	-0.61888600	0.59990000	-0.04046600
N	0.91709100	2.66613900	-1.81533400
C	2.17008300	3.10132700	-2.12590800
N	1.03918300	1.62177300	-1.01213200
C	2.63796300	4.17103600	-2.91771800
C	4.00918400	4.33731900	-2.97982600
H	1.93779300	4.83187900	-3.43267300
Zn	-2.16263600	1.48390000	3.06389100
Cl	-3.10939100	2.06892400	4.94422600
N	-2.17125000	2.82811100	1.54496600
C	-2.67464300	4.09179700	1.45142900
N	-1.59578300	2.53399100	0.39248500
C	-3.38412400	4.88318400	2.37351300
C	-3.76675300	6.15676800	1.95924200
H	-3.63273500	4.48024300	3.35671900

Ni	2.87310100	-0.19286000	0.31078500
N	1.65868100	0.39254400	2.04534000
C	1.94952700	0.60307900	3.36854800
N	0.36608800	0.64654800	1.89198100
C	3.16852100	0.53148700	4.06350000
C	3.15837400	0.84905700	5.41848700
N	-1.69075800	3.53588600	-0.46357500
C	-2.36337000	4.54908700	0.15099600
C	-2.74413700	5.83758500	-0.27869000
C	-3.43301700	6.61095100	0.63605900
H	-2.48947700	6.19144900	-1.27964400
N	2.31884000	1.30516800	-0.78787100
C	3.06780400	2.24409300	-1.45014800
C	4.46107900	2.42117400	-1.52126100
C	4.93432700	3.48473200	-2.28646400
H	5.13789600	1.74534800	-0.99511000
N	-0.21114800	0.99993000	3.03235300
C	0.74701700	0.99163900	4.00078800
C	0.71814300	1.29647900	5.37839300
C	1.92193200	1.21567300	6.05416900
H	-0.21556300	1.57805900	5.86921000
N	-2.91048600	-0.09360100	2.03238100
C	-3.94507200	-0.94701400	2.27310300
N	-2.36359900	-0.43504800	0.87936900
C	-4.86523500	-1.04968700	3.33691100
C	-5.80257200	-2.06069600	3.24159700
H	-4.81725600	-0.36508700	4.18605900
Zn	-2.32605400	-2.23217900	-1.41703200
Cl	-3.38871200	-3.95383800	-2.24531300
N	-2.28290900	-0.51736500	-2.48638600
C	-2.79412200	-0.18928900	-3.70704700
N	-1.68954000	0.55446300	-1.99346700
C	-3.50643100	-0.94800100	-4.65330700
C	-3.89539600	-0.30317300	-5.82515400
N	-2.97957100	-1.47171800	0.34103700
C	-3.99008300	-1.84060000	1.17908900
C	-4.95089600	-2.86441400	1.08792600
C	-5.86768300	-2.97187700	2.13125300
H	-4.97102200	-3.51736200	0.21373400
N	-1.77604400	1.57906800	-2.82286000
C	-2.46588200	1.16809300	-3.92435900
C	-2.85344000	1.83056600	-5.10766000
C	-3.56046000	1.08028500	-6.02845800
H	-2.60816500	2.88266200	-5.26562900
N	-0.36153800	-2.36753300	-0.97427700
C	0.52734900	-3.39515100	-1.05636800
N	0.28705900	-1.31242300	-0.50253800
C	0.39297600	-4.73253100	-1.48382400
C	1.53113700	-5.51352400	-1.42523800
H	-0.56982200	-5.11532000	-1.82823200
N	1.56668100	-1.56633000	-0.27992700

C	1.76523500	-2.89273000	-0.59361000
C	2.91721400	-3.69901700	-0.53553800
C	2.79824000	-5.02040400	-0.95861200
H	3.85763900	-3.27768000	-0.18011400
H	-3.71193500	-2.00288900	-4.46366400
H	4.08144100	0.27137400	3.53094700
C	-4.52289800	7.04978900	2.87864200
C	-4.24066400	7.02884600	4.27933800
C	-5.51667400	7.90175200	2.39071800
C	-4.91539000	7.82135900	5.19625200
H	-3.44646000	6.37338200	4.64230800
C	-6.21011800	8.71067900	3.30362400
H	-5.78285100	7.93316800	1.33336700
C	-5.91199900	8.66722000	4.68350900
H	-4.67089500	7.78700000	6.25945800
H	-6.91751700	9.86056700	6.17404200
C	6.39795800	3.73770600	-2.36495700
C	6.99904600	4.14960700	-3.59269500
C	7.19785500	3.53782700	-1.23842800
C	8.36572500	4.35101200	-3.73094400
H	6.36105600	4.28272000	-4.46910500
C	8.58013700	3.72940900	-1.36171100
H	6.77675100	3.23062700	-0.28171900
C	9.15275900	4.12808700	-2.58927400
H	8.79889800	4.65141400	-4.68668400
H	11.27026300	4.42038600	-2.89370800
C	4.43147200	0.82290100	6.18893300
C	4.66550000	1.77639200	7.22604400
C	5.85123300	1.83427100	7.94561000
H	3.89029000	2.51353200	7.44482300
C	5.42747600	-0.10584800	5.87423900
C	6.83974100	0.89739100	7.60561000
H	6.00300600	2.58366300	8.72460400
C	6.63445400	-0.05779400	6.58530300
H	5.28482900	-0.86542200	5.10494600
C	-6.91825800	-4.02510500	2.09808200
C	-6.61058100	-5.31636600	1.56928900
C	-7.55034500	-6.33192900	1.49892300
H	-5.59178200	-5.51111300	1.22932800
C	-8.20651000	-3.75060400	2.57055600
C	-8.84565100	-6.05709300	1.97055400
H	-7.30294100	-7.31716000	1.10029600
C	-9.15249800	-4.78190800	2.49601800
H	-8.47074900	-2.76296300	2.95166100
H	-11.10018900	-4.22446000	3.24258500
C	-4.66188100	-1.04282000	-6.86416200
C	-4.41257100	-0.79740500	-8.24917900
C	-5.08892900	-1.46902300	-9.25529000
H	-3.64135300	-0.07445500	-8.52163400
C	-5.61906200	-1.98932500	-6.48168100
C	-6.05078100	-2.41957600	-8.87285900

H	-4.88431500	-1.28152900	-10.31068100
C	-6.29784600	-2.66586300	-7.50347100
H	-5.84051900	-2.17458200	-5.42955900
H	-7.74256800	-4.09600800	-6.77827500
C	3.97862800	-5.92612200	-0.92901200
C	4.91058400	-5.84153400	0.15060200
C	6.03473300	-6.64824400	0.22475100
H	4.71266300	-5.13041900	0.95483500
C	4.18232000	-6.85037600	-1.95967600
C	6.24259900	-7.57510900	-0.81137000
H	6.73648000	-6.58087500	1.05771800
C	5.32102300	-7.66333700	-1.87883200
H	3.49754900	-6.91231900	-2.80695900
H	5.52446100	-9.03352000	-3.53484200
N	7.24643000	-8.49527300	-1.02284000
N	7.00810900	-9.12100200	-2.11918500
N	5.85864800	-8.64457800	-2.66141000
N	-7.27176300	-3.62188500	-7.53978300
N	-7.59126400	-3.93891600	-8.81936300
N	-6.87568100	-3.23244500	-9.61948700
N	10.71471900	3.83389400	-1.00812600
N	9.59399700	3.56605300	-0.44022800
N	10.48567400	4.18052200	-2.29948300
N	-7.22648800	9.62261900	3.10603000
N	-7.55517000	10.12584600	4.24075500
N	-6.78413500	9.57339500	5.21189800
N	-9.97852700	-6.83925800	2.03025100
N	-10.93202300	-6.14558800	2.54046000
N	-10.47069000	-4.90284600	2.83093100
N	7.77373900	-0.82864300	6.47427400
N	8.63468700	-0.41739100	7.33337600
N	8.10506300	0.61834500	8.03315400
H	8.65947700	1.06315700	8.75478800
H	-6.51398800	-2.19297800	4.05910300
H	4.40992100	5.17328500	-3.55688400
H	1.46276300	-6.56286600	-1.71892800
H	1.93246800	1.42463500	7.12575800
H	-3.90231300	1.56457500	-6.94511000
H	-3.72034600	7.62493200	0.35140500
C	4.66100000	0.38221700	0.78397700
C	4.62621500	-0.99545100	1.34515100
H	4.58986100	-1.03682700	2.45054100
C	5.69629200	-1.95135000	0.80876100
H	6.69239400	-1.61721200	1.16116000
H	5.55194300	-2.99022700	1.16346200
H	5.71495000	-1.96002100	-0.29885700
H	3.57300600	-1.49413000	1.10640900
C	4.91781300	1.62542900	1.60782300
H	5.10931400	2.49338800	0.94939500
H	4.06971300	1.91208400	2.25414700
H	5.81233100	1.50596100	2.26027000

H 5.27187800 0.35680400 -0.13952900

TS-βH^c

Ni-MFU-4l

Zn	20.16909500	6.91015300	9.16923800
Cl	17.99963900	7.26822800	9.05809700
Zn	23.71140100	6.34874900	9.34748100
N	21.42940000	8.44631800	9.59696600
C	21.17603100	9.77183100	9.77406700
N	22.74520200	8.26243800	9.70689700
C	19.96578700	10.49495100	9.75034000
C	20.06103300	11.85588700	9.95828500
H	18.99501100	10.00950300	9.57512200
Zn	24.39754800	3.85191200	11.84745600
Cl	24.84705400	2.34282200	13.38252400
N	22.46953000	4.40588400	11.49351300
C	21.29084200	4.01611100	12.05713300
N	22.19902400	5.32067500	10.56517300
C	21.00174400	3.08440000	13.07481700
C	19.66885400	2.93264800	13.40416100
H	21.78403900	2.50484800	13.58485300
Ni	25.41196600	9.47049200	10.19109300
N	25.53782500	7.78777200	11.33993700
C	26.23404000	7.62351000	12.50786500
N	24.92639100	6.63295100	11.08361600
C	27.05625400	8.49830600	13.24777300
C	27.62193000	7.99123300	14.40042800
N	20.89074500	5.54993100	10.49394700
C	20.27242700	4.75417100	11.41062200
C	18.91276500	4.59740900	11.74827900
C	18.63435900	3.68394200	12.74474000
H	18.11249100	5.16484500	11.25267300
N	23.37536600	9.40591500	9.96474700
C	22.42623700	10.39431700	10.00240000
C	22.51275300	11.78770800	10.20737000
C	21.32783700	12.49402200	10.18280900
H	23.46287500	12.30874700	10.37612100
N	25.18806200	5.71940600	12.01587800
C	26.00879100	6.29442000	12.93636900
C	26.58678700	5.77774800	14.11366100
C	27.38987600	6.64074700	14.83282900
H	26.41535200	4.74504100	14.44906700
N	24.94753800	3.51151700	9.91333400
C	25.59230900	2.46468300	9.32471700
N	24.69762600	4.42052400	8.97438700
C	26.08144400	1.25167200	9.85094200
C	26.69469800	0.39912300	8.95386700
H	25.98645800	0.98892800	10.91402000
Zn	24.90441700	5.20484900	6.16183600
Cl	25.62517900	4.52345400	4.19463800

N	22.91832100	5.59385800	6.39481000
C	21.86094500	5.50706900	5.53974300
N	22.46426100	6.03044000	7.56672500
C	21.77899200	5.10882800	4.18974400
C	20.52256700	5.14415800	3.61987500
N	25.15131700	4.01640000	7.79061400
C	25.72368200	2.79023900	7.95465700
C	26.34964300	1.91803600	7.04101400
C	26.82651100	0.73154000	7.56058400
H	26.45678200	2.15841800	5.97396100
N	21.14978200	6.23319900	7.51955900
C	20.71917200	5.91939700	6.26554100
C	19.43763100	5.95421200	5.67891500
C	19.36007200	5.56301300	4.35664500
H	18.54373900	6.27438200	6.23250900
N	25.59559900	6.95154500	6.94263300
C	26.41354100	7.89704000	6.40357400
N	25.21542700	7.37752500	8.14702800
C	27.07542500	7.94489400	5.15926500
C	27.83084800	9.07222800	4.90908600
H	26.99732000	7.13298600	4.42203000
N	25.75764700	8.55349800	8.43760900
C	26.51244200	8.93746300	7.35785800
C	27.28099400	10.08956500	7.08569600
C	27.92776200	10.13568600	5.86827200
H	27.37335300	10.93367600	7.78207100
H	22.65945600	4.78875100	3.61497400
C	18.02496700	5.20552200	2.43870400
C	19.17695300	4.79108600	1.70995100
C	16.77319700	5.24010000	1.85264700
C	19.10378800	4.40256400	0.38066900
C	16.68071400	4.84887600	0.50466100
C	17.83046200	4.43985500	-0.20799400
H	20.01765300	4.09072600	-0.14221300
C	29.24417800	10.27161500	3.44437600
C	29.33801400	11.32886200	4.39567200
C	29.90403500	10.33220500	2.23078900
C	30.09228400	12.46760700	4.15463400
C	30.67350900	11.48047400	1.97009600
C	30.75894400	12.52229800	2.92099000
H	30.13657300	13.25760000	4.91609800
C	17.00998200	2.60873000	14.08183300
C	18.03365700	1.86450300	14.73596600
C	15.67066600	2.45867300	14.40868300
C	17.73948200	0.95285700	15.73287800
C	15.37891200	1.53185900	15.42118800
C	16.38562800	0.78809900	16.07732400
H	18.54130700	0.38800700	16.22614500
C	27.79687500	-1.65491100	8.56042900
C	27.92665100	-1.32470900	7.18059400
C	28.28075400	-2.84710500	9.06655800

C	28.54224700	-2.17748900	6.27668600
C	28.90828600	-3.72416800	8.16340300
C	29.03114300	-3.38564700	6.79687100
H	28.62022300	-1.88204900	5.22196500
O	28.48719000	9.15179100	3.70994500
O	28.67754700	11.25539800	5.59713200
H	29.82050600	9.50845200	1.50986400
N	31.43172400	11.82171900	0.86621800
N	31.57826500	13.43061700	2.30650400
N	31.96722500	12.98388700	1.07479100
O	27.18007200	-0.78690800	9.43478700
O	27.44074000	-0.13656100	6.69298300
H	28.17185900	-3.08509600	10.13276700
N	29.48085000	-4.96522100	8.36794600
N	29.68113200	-4.46931400	6.27067300
N	29.93852200	-5.40168000	7.23612600
C	29.00481200	8.35113800	16.28186500
C	28.77446800	7.01247300	16.71157300
C	29.81342000	9.22270400	16.99576900
C	29.34925500	6.51648100	17.86722300
C	30.39358000	8.71295000	18.16747900
C	30.17237000	7.38714200	18.60388400
H	29.16092800	5.48221000	18.18363800
O	27.96627900	6.16909100	15.98157300
O	28.42644400	8.83044800	15.13139300
H	29.96335400	10.24626700	16.62747600
N	31.22568200	9.21709600	19.13036700
N	30.87168100	7.18248900	19.77821600
N	31.49592400	8.27656000	20.08453000
H	27.25822300	9.53373700	12.94227500
O	18.12890100	5.58604800	3.75882700
O	20.41337600	4.76175300	2.30620600
H	15.89640000	5.56234300	2.42942000
N	17.33314100	4.14920400	-1.44973100
N	15.98413500	4.36206900	-1.49860400
N	15.58689500	4.77950300	-0.33712400
O	19.35628000	2.03520200	14.38903700
H	14.91500400	3.05309600	13.87817700
O	17.31849000	3.51080100	13.09366900
N	14.23188900	1.09433600	16.02663500
N	15.79171100	-0.03294000	17.01700100
N	14.50943200	0.15534700	16.97993600
C	18.97995400	13.94933100	10.13680200
C	20.23737600	14.58319600	10.35658400
C	17.80154300	14.67231500	10.11214400
C	20.34372700	15.95174400	10.55573500
C	17.89151100	16.06161800	10.31289800
C	19.14395800	16.67915400	10.52951500
H	21.33303300	16.39857300	10.72137200
O	18.90400200	12.58801600	9.94160400
O	21.39952200	13.85245500	10.37972600

H	16.84184200	14.16722300	9.94140000
N	16.90625300	17.03029700	10.34282200
N	17.46310600	18.18096800	10.55892100
N	18.81266500	17.99923100	10.67633900
H	31.63815800	10.14703600	19.21272300
H	13.26289400	1.36833200	15.85997300
H	29.97476500	-4.64859400	5.30973700
H	31.90877300	14.33766900	2.63772600
H	19.41342100	18.80571500	10.85046600
H	17.81855800	3.81607900	-2.28350600
C	27.81567500	12.50554800	10.35701300
H	28.92297900	12.46167600	10.35118900
C	27.20523500	11.48476600	11.25783000
H	26.81678100	9.94782200	10.43757300
H	27.52871500	13.54718200	10.65081800
C	25.72679100	11.19214300	11.19877700
C	24.96809600	11.26776700	12.51872500
H	25.36846000	10.55207100	13.26358800
H	25.06342700	12.28343200	12.96893600
H	23.89026800	11.04380800	12.40332500
H	27.46423500	12.39073200	9.30643800
H	25.27219900	11.84980400	10.42172000
H	27.74574600	11.23906500	12.18825400

Ni-CFA-1

Zn	-0.91253700	3.34505500	-2.32523100
Cl	-1.06731900	5.02562000	-3.70727800
Zn	-0.61697700	0.60684700	-0.04505600
N	0.91709100	2.66613900	-1.81533400
C	2.17008300	3.10132700	-2.12590800
N	1.03918300	1.62177300	-1.01213200
C	2.63796300	4.17103600	-2.91771800
C	4.00918400	4.33731900	-2.97982600
H	1.93779300	4.83187900	-3.43267300
Zn	-2.16521000	1.48473500	3.06270500
Cl	-3.10939100	2.06892400	4.94422600
N	-2.17125000	2.82811100	1.54496600
C	-2.67464300	4.09179700	1.45142900
N	-1.59578300	2.53399100	0.39248500
C	-3.38412400	4.88318400	2.37351300
C	-3.76675300	6.15676800	1.95924200
H	-3.63273500	4.48024300	3.35671900
Ni	2.87018000	-0.33862400	0.58595700
N	1.66184600	0.38440400	2.04533400
C	1.94952700	0.60307900	3.36854800
N	0.36608800	0.64654800	1.89198100
C	3.16852100	0.53148700	4.06350000
C	3.15837400	0.84905700	5.41848700
N	-1.69075800	3.53588600	-0.46357500
C	-2.36337000	4.54908700	0.15099600
C	-2.74413700	5.83758500	-0.27869000

C	-3.43301700	6.61095100	0.63605900
H	-2.48947700	6.19144900	-1.27964400
N	2.30988200	1.32480600	-0.75728000
C	3.06780400	2.24409300	-1.45014800
C	4.46107900	2.42117400	-1.52126100
C	4.93432700	3.48473200	-2.28646400
H	5.13789600	1.74534800	-0.99511000
N	-0.21114800	0.99993000	3.03235300
C	0.74701700	0.99163900	4.00078800
C	0.71814300	1.29647900	5.37839300
C	1.92193200	1.21567300	6.05416900
H	-0.21556300	1.57805900	5.86921000
N	-2.91048600	-0.09360100	2.03238100
C	-3.94507200	-0.94701400	2.27310300
N	-2.36359900	-0.43504800	0.87936900
C	-4.86523500	-1.04968700	3.33691100
C	-5.80257200	-2.06069600	3.24159700
H	-4.81725600	-0.36508700	4.18605900
Zn	-2.32861000	-2.23068400	-1.41745000
Cl	-3.38871200	-3.95383800	-2.24531300
N	-2.28290900	-0.51736500	-2.48638600
C	-2.79412200	-0.18928900	-3.70704700
N	-1.68954000	0.55446300	-1.99346700
C	-3.50643100	-0.94800100	-4.65330700
C	-3.89539600	-0.30317300	-5.82515400
N	-2.97957100	-1.47171800	0.34103700
C	-3.99008300	-1.84060000	1.17908900
C	-4.95089600	-2.86441400	1.08792600
C	-5.86768300	-2.97187700	2.13125300
H	-4.97102200	-3.51736200	0.21373400
N	-1.77604400	1.57906800	-2.82286000
C	-2.46588200	1.16809300	-3.92435900
C	-2.85344000	1.83056600	-5.10766000
C	-3.56046000	1.08028500	-6.02845800
H	-2.60816500	2.88266200	-5.26562900
N	-0.36153800	-2.36753300	-0.97427700
C	0.52734900	-3.39515100	-1.05636800
N	0.28705900	-1.31242300	-0.50253800
C	0.39297600	-4.73253100	-1.48382400
C	1.53113700	-5.51352400	-1.42523800
H	-0.56982200	-5.11532000	-1.82823200
N	1.56000000	-1.57781700	-0.24790900
C	1.76523500	-2.89273000	-0.59361000
C	2.91721400	-3.69901700	-0.53553800
C	2.79824000	-5.02040400	-0.95861200
H	3.85763900	-3.27768000	-0.18011400
H	-3.71193500	-2.00288900	-4.46366400
H	4.08144100	0.27137400	3.53094700
C	-4.52289800	7.04978900	2.87864200
C	-4.24066400	7.02884600	4.27933800
C	-5.51667400	7.90175200	2.39071800

C	-4.91539000	7.82135900	5.19625200
H	-3.44646000	6.37338200	4.64230800
C	-6.21011800	8.71067900	3.30362400
H	-5.78285100	7.93316800	1.33336700
C	-5.91199900	8.66722000	4.68350900
H	-4.67089500	7.78700000	6.25945800
H	-6.91751700	9.86056700	6.17404200
C	6.39795800	3.73770600	-2.36495700
C	6.99904600	4.14960700	-3.59269500
C	7.19785500	3.53782700	-1.23842800
C	8.36572500	4.35101200	-3.73094400
H	6.36105600	4.28272000	-4.46910500
C	8.58013700	3.72940900	-1.36171100
H	6.77675100	3.23062700	-0.28171900
C	9.15275900	4.12808700	-2.58927400
H	8.79889800	4.65141400	-4.68668400
H	11.27026300	4.42038600	-2.89370800
C	4.43147200	0.82290100	6.18893300
C	4.66550000	1.77639200	7.22604400
C	5.85123300	1.83427100	7.94561000
H	3.89029000	2.51353200	7.44482300
C	5.42747600	-0.10584800	5.87423900
C	6.83974100	0.89739100	7.60561000
H	6.00300600	2.58366300	8.72460400
C	6.63445400	-0.05779400	6.58530300
H	5.28482900	-0.86542200	5.10494600
C	-6.91825800	-4.02510500	2.09808200
C	-6.61058100	-5.31636600	1.56928900
C	-7.55034500	-6.33192900	1.49892300
H	-5.59178200	-5.51111300	1.22932800
C	-8.20651000	-3.75060400	2.57055600
C	-8.84565100	-6.05709300	1.97055400
H	-7.30294100	-7.31716000	1.10029600
C	-9.15249800	-4.78190800	2.49601800
H	-8.47074900	-2.76296300	2.95166100
H	-11.10018900	-4.22446000	3.24258500
C	-4.66188100	-1.04282000	-6.86416200
C	-4.41257100	-0.79740500	-8.24917900
C	-5.08892900	-1.46902300	-9.25529000
H	-3.64135300	-0.07445500	-8.52163400
C	-5.61906200	-1.98932500	-6.48168100
C	-6.05078100	-2.41957600	-8.87285900
H	-4.88431500	-1.28152900	-10.31068100
C	-6.29784600	-2.66586300	-7.50347100
H	-5.84051900	-2.17458200	-5.42955900
H	-7.74256800	-4.09600800	-6.77827500
C	3.97862800	-5.92612200	-0.92901200
C	4.91058400	-5.84153400	0.15060200
C	6.03473300	-6.64824400	0.22475100
H	4.71266300	-5.13041900	0.95483500
C	4.18232000	-6.85037600	-1.95967600

C	6.24259900	-7.57510900	-0.81137000
H	6.73648000	-6.58087500	1.05771800
C	5.32102300	-7.66333700	-1.87883200
H	3.49754900	-6.91231900	-2.80695900
H	5.52446100	-9.03352000	-3.53484200
N	7.24643000	-8.49527300	-1.02284000
N	7.00810900	-9.12100200	-2.11918500
N	5.85864800	-8.64457800	-2.66141000
N	-7.27176300	-3.62188500	-7.53978300
N	-7.59126400	-3.93891600	-8.81936300
N	-6.87568100	-3.23244500	-9.61948700
N	10.71471900	3.83389400	-1.00812600
N	9.59399700	3.56605300	-0.44022800
N	10.48567400	4.18052200	-2.29948300
N	-7.22648800	9.62261900	3.10603000
N	-7.55517000	10.12584600	4.24075500
N	-6.78413500	9.57339500	5.21189800
N	-9.97852700	-6.83925800	2.03025100
N	-10.93202300	-6.14558800	2.54046000
N	-10.47069000	-4.90284600	2.83093100
N	7.77373900	-0.82864300	6.47427400
N	8.63468700	-0.41739100	7.33337600
N	8.10506300	0.61834500	8.03315400
H	8.65947700	1.06315700	8.75478800
H	-6.51398800	-2.19297800	4.05910300
H	4.40992100	5.17328500	-3.55688400
H	1.46276300	-6.56286600	-1.71892800
H	1.93246800	1.42463500	7.12575800
H	-3.90231300	1.56457500	-6.94511000
H	-3.72034600	7.62493200	0.35140500
C	4.76292300	0.28349800	0.89520700
C	4.70560200	-0.87283800	0.00639000
H	5.33235300	-1.69972200	0.41274500
C	4.76781200	-0.88772800	-1.51423800
H	5.80907800	-0.68808900	-1.84985300
H	4.48725100	-1.88718700	-1.90041300
H	4.10090000	-0.15047800	-1.99158500
H	3.65769900	-1.56314400	0.75975300
C	5.70968200	0.20191100	2.07056100
H	6.75252500	0.26140900	1.68411100
H	5.60102300	1.04143200	2.78212100
H	5.63691700	-0.75497700	2.62713700
H	4.69052500	1.29891300	0.49564200

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Ni-MFU-4l

Zn	20.17032200	6.91033000	9.16951600
Cl	17.99963900	7.26822800	9.05809700
Zn	23.71695700	6.35273800	9.34961000
N	21.42940000	8.44631800	9.59696800

C	21.17603100	9.77183100	9.77406900
N	22.74520200	8.26243700	9.70689800
C	19.96578700	10.49495100	9.75034100
C	20.06103300	11.85588700	9.95828500
H	18.99501100	10.00950300	9.57512200
Zn	24.40099600	3.85598800	11.84838200
Cl	24.84705400	2.34282200	13.38252400
N	22.46953000	4.40588400	11.49351300
C	21.29084200	4.01611100	12.05713300
N	22.19902400	5.32067500	10.56517300
C	21.00174400	3.08440000	13.07481700
C	19.66885400	2.93264800	13.40416100
H	21.78403900	2.50484800	13.58485300
Ni	25.36694300	9.45295200	10.14352600
N	25.51873900	7.79293900	11.35873000
C	26.23403600	7.62351200	12.50786000
N	24.92638800	6.63295300	11.08361300
C	27.05625400	8.49830600	13.24777300
C	27.62193000	7.99123300	14.40042800
N	20.89074500	5.54993100	10.49394700
C	20.27242700	4.75417100	11.41062200
C	18.91276500	4.59740900	11.74827900
C	18.63435900	3.68394200	12.74474000
H	18.11249100	5.16484500	11.25267300
N	23.38617600	9.41210600	9.95137200
C	22.42623700	10.39431500	10.00240400
C	22.51275300	11.78770800	10.20737100
C	21.32783700	12.49402200	10.18281000
H	23.46287500	12.30874700	10.37612000
N	25.18806100	5.71940700	12.01587900
C	26.00879000	6.29442000	12.93636900
C	26.58678700	5.77774800	14.11366100
C	27.38987600	6.64074700	14.83282900
H	26.41535200	4.74504100	14.44906700
N	24.94753800	3.51151700	9.91333400
C	25.59230900	2.46468300	9.32471700
N	24.69762600	4.42052400	8.97438700
C	26.08144400	1.25167200	9.85094200
C	26.69469800	0.39912300	8.95386700
H	25.98645800	0.98892800	10.91402000
Zn	24.90700000	5.20790300	6.16322100
Cl	25.62517900	4.52345400	4.19463800
N	22.91832100	5.59385800	6.39481000
C	21.86094500	5.50706900	5.53974300
N	22.46426100	6.03044000	7.56672500
C	21.77899200	5.10882800	4.18974400
C	20.52256700	5.14415800	3.61987500
N	25.15131700	4.01640000	7.79061400
C	25.72368200	2.79023900	7.95465700
C	26.34964300	1.91803600	7.04101400
C	26.82651100	0.73154000	7.56058400

H	26.45678200	2.15841800	5.97396100
N	21.14978200	6.23319900	7.51955900
C	20.71917200	5.91939700	6.26554100
C	19.43763100	5.95421200	5.67891500
C	19.36007200	5.56301300	4.35664500
H	18.54373900	6.27438200	6.23250900
N	25.59560000	6.95154400	6.94263400
C	26.41354300	7.89703900	6.40357400
N	25.21543000	7.37752500	8.14702700
C	27.07542500	7.94489400	5.15926500
C	27.83084800	9.07222800	4.90908600
H	26.99732000	7.13298600	4.42203000
N	25.73363100	8.57458800	8.41503200
C	26.51244600	8.93746200	7.35785600
C	27.28099500	10.08956500	7.08569600
C	27.92776200	10.13568600	5.86827200
H	27.37335300	10.93367600	7.78207100
H	22.65945600	4.78875100	3.61497400
C	18.02496700	5.20552200	2.43870400
C	19.17695300	4.79108600	1.70995100
C	16.77319700	5.24010000	1.85264700
C	19.10378800	4.40256400	0.38066900
C	16.68071400	4.84887600	0.50466100
C	17.83046200	4.43985500	-0.20799400
H	20.01765300	4.09072600	-0.14221300
C	29.24417800	10.27161500	3.44437600
C	29.33801400	11.32886200	4.39567200
C	29.90403500	10.33220500	2.23078900
C	30.09228400	12.46760700	4.15463400
C	30.67350900	11.48047400	1.97009600
C	30.75894400	12.52229800	2.92099000
H	30.13657300	13.25760000	4.91609800
C	17.00998200	2.60873000	14.08183300
C	18.03365700	1.86450300	14.73596600
C	15.67066600	2.45867300	14.40868300
C	17.73948200	0.95285700	15.73287800
C	15.37891200	1.53185900	15.42118800
C	16.38562800	0.78809900	16.07732400
H	18.54130700	0.38800700	16.22614500
C	27.79687500	-1.65491100	8.56042900
C	27.92665100	-1.32470900	7.18059400
C	28.28075400	-2.84710500	9.06655800
C	28.54224700	-2.17748900	6.27668600
C	28.90828600	-3.72416800	8.16340300
C	29.03114300	-3.38564700	6.79687100
H	28.62022300	-1.88204900	5.22196500
O	28.48719000	9.15179100	3.70994500
O	28.67754700	11.25539800	5.59713200
H	29.82050600	9.50845200	1.50986400
N	31.43172400	11.82171900	0.86621800
N	31.57826500	13.43061700	2.30650400

N	31.96722500	12.98388700	1.07479100
O	27.18007200	-0.78690800	9.43478700
O	27.44074000	-0.13656100	6.69298300
H	28.17185900	-3.08509600	10.13276700
N	29.48085000	-4.96522100	8.36794600
N	29.68113200	-4.46931400	6.27067300
N	29.93852200	-5.40168000	7.23612600
C	29.00481200	8.35113800	16.28186500
C	28.77446800	7.01247300	16.71157300
C	29.81342000	9.22270400	16.99576900
C	29.34925500	6.51648100	17.86722300
C	30.39358000	8.71295000	18.16747900
C	30.17237000	7.38714200	18.60388400
H	29.16092800	5.48221000	18.18363800
O	27.96627900	6.16909100	15.98157300
O	28.42644400	8.83044800	15.13139300
H	29.96335400	10.24626700	16.62747600
N	31.22568200	9.21709600	19.13036700
N	30.87168100	7.18248900	19.77821600
N	31.49592400	8.27656000	20.08453000
H	27.25822300	9.53373700	12.94227500
O	18.12890100	5.58604800	3.75882700
O	20.41337600	4.76175300	2.30620600
H	15.89640000	5.56234300	2.42942000
N	17.33314100	4.14920400	-1.44973100
N	15.98413500	4.36206900	-1.49860400
N	15.58689500	4.77950300	-0.33712400
O	19.35628000	2.03520200	14.38903700
H	14.91500400	3.05309600	13.87817700
O	17.31849000	3.51080100	13.09366900
N	14.23188900	1.09433600	16.02663500
N	15.79171100	-0.03294000	17.01700100
N	14.50943200	0.15534700	16.97993600
C	18.97995400	13.94933100	10.13680200
C	20.23737600	14.58319600	10.35658400
C	17.80154300	14.67231500	10.11214400
C	20.34372700	15.95174400	10.55573500
C	17.89151100	16.06161800	10.31289800
C	19.14395800	16.67915400	10.52951500
H	21.33303300	16.39857300	10.72137200
O	18.90400200	12.58801600	9.94160400
O	21.39952200	13.85245500	10.37972600
H	16.84184200	14.16722300	9.94140000
N	16.90625300	17.03029700	10.34282200
N	17.46310600	18.18096800	10.55892100
N	18.81266500	17.99923100	10.67633900
H	31.63815800	10.14703600	19.21272300
H	13.26289400	1.36833200	15.85997300
H	29.97476500	-4.64859400	5.30973700
H	31.90877300	14.33766900	2.63772600
H	19.41342100	18.80571500	10.85046600

H	17.81855800	3.81607900	-2.28350600
C	27.43861800	11.97195400	9.93026300
H	28.35746600	11.50769400	9.52489900
C	26.74872100	11.12903200	10.96086500
H	26.66877200	8.86663300	10.09466900
H	27.75033000	12.91207800	10.43614700
C	25.41543500	11.12700600	11.25504100
C	24.77370200	10.96487400	12.62046500
H	25.28698800	10.20576200	13.23905500
H	24.79749700	11.92712100	13.17418400
H	23.71642500	10.65509600	12.53295300
H	26.77436600	12.26581600	9.10181700
H	24.85453600	11.72461800	10.51478900
H	27.45400900	10.65226600	11.66653100

Ni-CFA-1

Zn	-0.91745500	3.34516000	-2.32557600
Cl	-1.06732400	5.02561900	-3.70727600
Zn	-0.62452700	0.59942800	-0.04893500
N	0.91714400	2.66618100	-1.81529700
C	2.17011600	3.10134300	-2.12593600
N	1.03909700	1.62192700	-1.01194900
C	2.63796200	4.17105500	-2.91769300
C	4.00918400	4.33731900	-2.97982600
H	1.93779300	4.83187900	-3.43267300
Zn	-2.16783800	1.48437700	3.06212500
Cl	-3.10939000	2.06892800	4.94422500
N	-2.17125000	2.82811000	1.54496400
C	-2.67464100	4.09179800	1.45143000
N	-1.59577900	2.53397800	0.39246500
C	-3.38412400	4.88318400	2.37351300
C	-3.76675300	6.15676800	1.95924200
H	-3.63273500	4.48024300	3.35671900
Ni	2.86222600	-0.27857400	0.56929500
N	1.66107100	0.40697200	2.04089900
C	1.94951800	0.60306500	3.36854100
N	0.36610200	0.64654900	1.89197600
C	3.16852100	0.53148700	4.06350000
C	3.15837500	0.84906000	5.41848600
N	-1.69074800	3.53586900	-0.46358800
C	-2.36337500	4.54908500	0.15099500
C	-2.74413600	5.83758600	-0.27869000
C	-3.43301700	6.61095100	0.63605900
H	-2.48947700	6.19144900	-1.27964400
N	2.31267500	1.32114300	-0.75671600
C	3.06781400	2.24382700	-1.45032500
C	4.46107000	2.42125200	-1.52123300
C	4.93432500	3.48475800	-2.28642800
H	5.13789600	1.74534800	-0.99511000
N	-0.21115200	0.99992800	3.03235200

C	0.74701900	0.99164400	4.00078900
C	0.71814300	1.29648000	5.37839300
C	1.92193200	1.21567300	6.05416900
H	-0.21556300	1.57805900	5.86921000
N	-2.91048200	-0.09360400	2.03238600
C	-3.94507400	-0.94701200	2.27310200
N	-2.36360400	-0.43505000	0.87936100
C	-4.86523500	-1.04968700	3.33691100
C	-5.80257200	-2.06069600	3.24159700
H	-4.81725600	-0.36508700	4.18605900
Zn	-2.32540000	-2.23343700	-1.41733700
Cl	-3.38871500	-3.95383600	-2.24531400
N	-2.28290900	-0.51737600	-2.48636500
C	-2.79411700	-0.18929300	-3.70705000
N	-1.68955300	0.55444300	-1.99347100
C	-3.50643100	-0.94800100	-4.65330700
C	-3.89539600	-0.30317300	-5.82515400
N	-2.97958300	-1.47171900	0.34105700
C	-3.99008300	-1.84059800	1.17909000
C	-4.95089700	-2.86441300	1.08792500
C	-5.86768300	-2.97187700	2.13125300
H	-4.97102200	-3.51736200	0.21373400
N	-1.77604700	1.57905500	-2.82287700
C	-2.46587500	1.16809100	-3.92436200
C	-2.85344200	1.83056600	-5.10765900
C	-3.56046000	1.08028500	-6.02845800
H	-2.60816500	2.88266200	-5.26562900
N	-0.36155700	-2.36754300	-0.97423100
C	0.52736600	-3.39518600	-1.05636900
N	0.28708800	-1.31246300	-0.50265000
C	0.39297200	-4.73253600	-1.48380800
C	1.53113700	-5.51352400	-1.42523800
H	-0.56982200	-5.11532000	-1.82823200
N	1.56032900	-1.57689500	-0.25943600
C	1.76525000	-2.89258800	-0.59366000
C	2.91718000	-3.69906200	-0.53547600
C	2.79824200	-5.02040100	-0.95862100
H	3.85764400	-3.27767500	-0.18013300
H	-3.71193500	-2.00288900	-4.46366400
H	4.08144100	0.27137300	3.53094700
C	-4.52289800	7.04978900	2.87864200
C	-4.24066400	7.02884600	4.27933800
C	-5.51667400	7.90175200	2.39071800
C	-4.91539000	7.82135900	5.19625200
H	-3.44646000	6.37338200	4.64230800
C	-6.21011800	8.71067900	3.30362400
H	-5.78285100	7.93316800	1.33336700
C	-5.91199900	8.66722000	4.68350900
H	-4.67089500	7.78700000	6.25945800
H	-6.91751700	9.86056700	6.17404200
C	6.39795800	3.73770600	-2.36495700

C	6.99904600	4.14960700	-3.59269500
C	7.19785500	3.53782700	-1.23842800
C	8.36572500	4.35101200	-3.73094400
H	6.36105600	4.28272000	-4.46910500
C	8.58013700	3.72940900	-1.36171100
H	6.77675100	3.23062700	-0.28171900
C	9.15275900	4.12808700	-2.58927400
H	8.79889800	4.65141400	-4.68668400
H	11.27026300	4.42038600	-2.89370800
C	4.43147200	0.82290100	6.18893300
C	4.66550000	1.77639200	7.22604400
C	5.85123300	1.83427100	7.94561000
H	3.89029000	2.51353200	7.44482300
C	5.42747600	-0.10584800	5.87423900
C	6.83974100	0.89739100	7.60561000
H	6.00300600	2.58366300	8.72460400
C	6.63445400	-0.05779400	6.58530300
H	5.28482900	-0.86542200	5.10494600
C	-6.91825800	-4.02510500	2.09808200
C	-6.61058100	-5.31636600	1.56928900
C	-7.55034500	-6.33192900	1.49892300
H	-5.59178200	-5.51111300	1.22932800
C	-8.20651000	-3.75060400	2.57055600
C	-8.84565100	-6.05709300	1.97055400
H	-7.30294100	-7.31716000	1.10029600
C	-9.15249800	-4.78190800	2.49601800
H	-8.47074900	-2.76296300	2.95166100
H	-11.10018900	-4.22446000	3.24258500
C	-4.66188100	-1.04282000	-6.86416200
C	-4.41257100	-0.79740500	-8.24917900
C	-5.08892900	-1.46902300	-9.25529000
H	-3.64135300	-0.07445500	-8.52163400
C	-5.61906200	-1.98932500	-6.48168100
C	-6.05078100	-2.41957600	-8.87285900
H	-4.88431500	-1.28152900	-10.31068100
C	-6.29784600	-2.66586300	-7.50347100
H	-5.84051900	-2.17458200	-5.42955900
H	-7.74256800	-4.09600800	-6.77827500
C	3.97862800	-5.92612200	-0.92901200
C	4.91058400	-5.84153400	0.15060200
C	6.03473300	-6.64824400	0.22475100
H	4.71266300	-5.13041900	0.95483500
C	4.18232000	-6.85037600	-1.95967600
C	6.24259900	-7.57510900	-0.81137000
H	6.73648000	-6.58087500	1.05771800
C	5.32102300	-7.66333700	-1.87883200
H	3.49754900	-6.91231900	-2.80695900
H	5.52446100	-9.03352000	-3.53484200
N	7.24643000	-8.49527300	-1.02284000
N	7.00810900	-9.12100200	-2.11918500
N	5.85864800	-8.64457800	-2.66141000

N	-7.27176300	-3.62188500	-7.53978300
N	-7.59126400	-3.93891600	-8.81936300
N	-6.87568100	-3.23244500	-9.61948700
N	10.71471900	3.83389400	-1.00812600
N	9.59399700	3.56605300	-0.44022800
N	10.48567400	4.18052200	-2.29948300
N	-7.22648800	9.62261900	3.10603000
N	-7.55517000	10.12584600	4.24075500
N	-6.78413500	9.57339500	5.21189800
N	-9.97852700	-6.83925800	2.03025100
N	-10.93202300	-6.14558800	2.54046000
N	-10.47069000	-4.90284600	2.83093100
N	7.77373900	-0.82864300	6.47427400
N	8.63468700	-0.41739100	7.33337600
N	8.10506300	0.61834500	8.03315400
H	8.65947700	1.06315700	8.75478800
H	-6.51398800	-2.19297800	4.05910300
H	4.40992100	5.17328500	-3.55688400
H	1.46276300	-6.56286600	-1.71892800
H	1.93246800	1.42463500	7.12575800
H	-3.90231300	1.56457500	-6.94511000
H	-3.72034600	7.62493200	0.35140500
C	4.82486000	0.16737500	0.76982800
C	4.60210727	-0.79801152	-0.21421623
H	4.94392227	-1.78821252	0.14459977
C	4.62726727	-0.74395252	-1.72524023
H	5.67687727	-0.66478752	-2.08828923
H	4.21552627	-1.68781752	-2.13486023
H	4.05539927	0.08412848	-2.17334723
H	3.18861200	-1.30786000	1.49168400
C	5.72981600	-0.17680000	1.93472400
H	5.69865500	0.57489200	2.74614200
H	5.52030400	-1.17620600	2.36655700
H	6.78305500	-0.18967000	1.57744600
H	4.84142500	1.23990100	0.53758300

TS-cw

Ni-MFU-4l

Zn	22.52313800	11.04635400	6.07441700
Cl	21.32696700	12.34850300	4.78837600
Zn	24.48325500	8.96229000	8.19359900
N	23.77796900	11.85784900	7.43384800
C	24.01180700	13.15823300	7.74122300
N	24.53854400	11.11347100	8.22395100
C	23.46552400	14.34288000	7.20570100
C	23.90703200	15.52768900	7.75666000
H	22.73013200	14.32949300	6.39980300
Zn	22.28465200	6.85350900	10.09745900
Cl	20.96096400	5.58493900	11.29035300
N	21.47004200	8.18145100	8.80253100
C	20.18155800	8.46878100	8.47236100

N	22.26068200	8.95808300	8.08011000
C	18.95507900	7.94573800	8.93049100
C	17.81358200	8.48079400	8.36617000
H	18.89951100	7.16241800	9.68761600
Ni	26.47494400	11.00635000	10.46781700
N	25.15152900	9.63813200	11.11660500
C	24.83193600	9.31494000	12.40785300
N	24.38349200	8.88102100	10.34044200
C	25.31692700	9.79208800	13.64329600
C	24.76017400	9.24911000	14.78327000
N	21.55765000	9.74732300	7.28597300
C	20.23879900	9.48385800	7.48978100
C	19.07226900	10.02879300	6.91556500
C	17.87404400	9.51393700	7.36710500
H	19.10518700	10.81282300	6.15791500
N	25.26641900	11.85119100	9.06159600
C	24.96792000	13.15785900	8.78392800
C	25.40017400	14.37945400	9.34360600
C	24.86696800	15.54001100	8.82166300
H	26.11473900	14.44745700	10.15638000
N	23.57278700	8.10088600	11.04226500
C	23.81730100	8.33125900	12.35816800
C	23.24708500	7.77781100	13.52289300
C	23.73207700	8.24818200	14.72665200
H	22.46425700	7.01887200	13.48405300
N	23.60955000	5.97919700	8.83532400
C	23.86890900	4.67670900	8.54033400
N	24.43355700	6.73131400	8.12567000
C	23.29480700	3.47594200	9.00562600
C	23.81388000	2.30763500	8.48304900
H	22.48651200	3.45975100	9.73798800
Zn	26.58883200	6.91030000	6.19062500
Cl	27.90469500	5.65650100	4.96347300
N	25.36149500	8.21507500	5.25195800
C	25.14624500	8.50708900	3.94112900
N	24.56081700	8.97555700	5.97800800
C	25.72168300	7.99979900	2.75831400
C	25.25622000	8.53773800	1.57561000
N	25.22799900	5.98949000	7.37274500
C	24.91800700	4.68358000	7.59222800
C	25.44654300	3.48948000	7.06084600
C	24.88108800	2.31666400	7.51873000
H	26.25617200	3.48262300	6.32999500
N	23.82255000	9.76012900	5.21076900
C	24.14889400	9.50900000	3.91407500
C	23.67680800	10.05591900	2.70345600
C	24.24238700	9.55761900	1.54613800
H	22.90919400	10.83025300	2.67179100
N	27.38589900	8.16109600	7.57548600
C	28.68367300	8.32035700	7.93449100
N	26.65415300	8.96370200	8.33194200

C	29.84825700	7.69803500	7.43911900
C	31.04050600	8.06976400	8.02213400
H	29.81269000	6.95936000	6.63689300
N	27.39532700	9.66334000	9.18240700
C	28.69798000	9.28324300	8.97207900
C	29.93234000	9.64169300	9.56182300
C	31.07354100	9.03535000	9.07955500
H	30.03405200	10.35782500	10.36870500
H	26.49105400	7.22667700	2.76737000
C	24.35627200	9.59226000	-0.81496200
C	25.36023900	8.58165900	-0.78457300
C	23.90372700	10.12526400	-2.00774000
C	25.93353200	8.08187700	-1.94426000
C	24.47451300	9.62952800	-3.19402600
C	25.46956500	8.62705500	-3.15125300
H	26.69887900	7.30868400	-1.87579600
C	33.38813800	7.85500100	8.14605600
C	33.42249800	8.81518600	9.19923200
C	34.54412100	7.26215900	7.67253300
C	34.61125100	9.20225800	9.80000800
C	35.75851000	7.64344900	8.27114600
C	35.78012400	8.59633300	9.31431200
H	34.59324400	9.94017700	10.60215800
C	15.51408300	9.53338000	7.25322200
C	15.45288700	8.51001200	8.24267400
C	14.37046100	10.07268500	6.68357900
C	14.24460200	8.00349900	8.68433600
C	13.14758000	9.55415800	7.13630400
C	13.07418500	8.53945700	8.11709900
H	14.21851400	7.22056300	9.44212200
C	23.77874800	-0.05512300	8.41114500
C	24.83601900	-0.04499100	7.45601400
C	23.22395700	-1.23862500	8.86196000
C	25.36174400	-1.21597200	6.93089600
C	23.74540300	-2.43614500	8.33956600
C	24.79415700	-2.41340400	7.39271700
H	26.17070200	-1.16290100	6.20216800
O	32.19316400	7.49423900	7.57312100
O	32.26663700	9.39051500	9.65382100
H	34.49730900	6.53008700	6.86643500
N	37.05047000	7.23846800	8.02326300
N	37.10784200	8.68782100	9.61330300
N	37.84020000	7.86236100	8.82247000
O	23.28335400	1.12528500	8.90936900
O	25.36995800	1.13851700	7.02386000
H	22.41564500	-1.22565700	9.59297300
N	23.40961900	-3.74779800	8.58726600
N	25.00653300	-3.73766400	7.14439100
N	24.16164300	-4.50895000	7.87522000
C	24.68425400	9.18669800	17.14424300
C	23.66510400	8.19208600	17.08806800

C	25.17150400	9.67052500	18.34935600
C	23.11205000	7.66011200	18.23843900
C	24.60575400	9.12621000	19.51253200
C	23.59514600	8.13951900	19.46938300
H	22.33334100	6.90016100	18.17499400
O	23.20597200	7.73603000	15.87706100
O	25.21903900	9.69958400	15.99301900
H	25.95150800	10.43201300	18.34767200
N	24.78877500	9.31390000	20.85112500
N	23.25028000	7.81153200	20.76097800
N	23.96208700	8.51178000	21.56990100
H	26.08751100	10.55565400	13.72403800
O	23.81081300	10.06292000	0.35474200
O	25.79288000	8.06849700	0.40785500
H	23.13498000	10.89787000	-2.01023200
N	25.75469600	8.42719100	-4.47003400
N	25.00044600	9.23657700	-5.25660100
N	24.23796000	9.95361500	-4.51064400
O	16.60775400	7.99980000	8.78455100
H	14.46255300	10.85439500	5.92944100
O	16.72153800	10.01980400	6.83136700
N	11.83572300	9.79404600	6.85020700
N	11.74841600	8.24835600	8.34532700
N	11.02486300	8.99610900	7.59079700
C	23.82450300	17.88742500	7.80857900
C	24.77652600	17.90025200	8.86936700
C	23.29923600	19.05970900	7.29675100
C	25.22276500	19.08295800	9.44021100
C	23.74126000	20.26837800	7.86438600
C	24.68531400	20.26847300	8.91578200
H	25.95187400	19.04814400	10.24981900
O	23.40416500	16.69777600	7.26656700
O	25.28496300	16.72826500	9.36139100
H	22.57223600	19.02943100	6.48528400
N	23.40920700	21.57272000	7.57610200
N	24.06833500	22.35021100	8.35878200
N	24.84628200	21.59733100	9.17809100
H	25.42256000	9.93636000	21.33756300
H	11.42496400	10.45012200	6.19693300
H	25.67255300	-4.18142300	6.52361200
H	37.57828700	9.25784900	10.30581500
H	25.43512200	22.05601300	9.86268400
H	26.41552200	7.79170400	-4.90058300
C	27.83601900	11.44351600	11.84252400
H	27.80251300	12.08225100	12.74943500
C	28.12286200	12.12964200	10.59288100
H	28.78613300	11.64806700	9.86339900
H	28.27818100	10.45421900	12.06463200
C	28.30096500	13.62857100	10.58727200
H	28.07156700	14.04043800	9.58389700
H	27.60612600	14.10859300	11.31001800

C	29.74683100	14.00201400	10.95859300
H	30.47041500	13.55821700	10.24427500
H	29.89135300	15.10114100	10.94581000
H	30.00971300	13.63376800	11.97158600
H	26.38694800	11.59670400	11.82379000

Ni-CFA-1

Zn	-0.33590700	3.61355500	-2.62788600
Cl	-0.58848600	5.28440600	-4.03007000
Zn	0.08128900	0.86288700	-0.31728900
N	1.51336300	2.88130600	-2.23166900
C	2.76319300	3.33624800	-2.53421000
N	1.66755400	1.73546400	-1.55832200
C	3.16633800	4.30286200	-3.47907600
C	4.52477000	4.41669000	-3.70399100
H	2.42199200	4.91109800	-4.01427300
Zn	-1.50194000	1.75054700	2.81424500
Cl	-2.45120100	2.30327600	4.72024800
N	-1.51895700	3.09343400	1.28765900
C	-2.09218300	4.33218700	1.17575000
N	-0.91371000	2.80992000	0.13668200
C	-2.81273600	5.11421100	2.09702600
C	-3.22554500	6.37659600	1.67686700
H	-3.04599200	4.71658100	3.09565600
Ni	3.56868400	0.13395000	0.26748600
N	2.33276300	0.59808400	1.81099900
C	2.58315600	0.74283800	3.15658000
N	1.04129100	0.84743300	1.63113400
C	3.73115000	0.44818400	3.91516500
C	3.64153900	0.56766100	5.29903600
N	-1.06401600	3.80431700	-0.73272300
C	-1.79875200	4.78738600	-0.12941000
C	-2.21032600	6.06409600	-0.56502200
C	-2.91029200	6.82888300	0.34880300
H	-1.96480800	6.42259900	-1.57541300
N	2.95482200	1.53243400	-1.23348600
C	3.70149200	2.52935800	-1.85142600
C	5.08124600	2.64442100	-2.10852900
C	5.49587500	3.60061300	-3.03157200
H	5.80506300	1.90039900	-1.76855400
N	0.44866600	1.22440500	2.76910500
C	1.37074500	1.12912300	3.77231200
C	1.26603900	1.25717700	5.17329900
C	2.40496200	0.97825800	5.90452600
H	0.31277000	1.54088000	5.64322300
N	-2.18989400	0.14524400	1.77225100
C	-3.18852900	-0.75047000	2.02062200
N	-1.61400400	-0.19037800	0.62315300
C	-4.12264400	-0.86430200	3.07121600
C	-5.02974400	-1.90237200	2.97541200

H	-4.11060800	-0.16215600	3.91766400
Zn	-1.51564700	-2.05699700	-1.64557600
Cl	-2.52021100	-3.83718200	-2.46160400
N	-1.55431100	-0.32223900	-2.70325600
C	-2.06749400	-0.02429700	-3.93094900
N	-1.02447500	0.78797700	-2.20481800
C	-2.76666100	-0.81719900	-4.85896400
C	-3.20435800	-0.19607000	-6.02635000
N	-2.18768400	-1.26767200	0.10074500
C	-3.18968800	-1.66059300	0.93957200
C	-4.12035400	-2.71204500	0.84756800
C	-5.05120000	-2.83018100	1.87710800
H	-4.11341800	-3.38377500	-0.02341300
N	-1.15397700	1.80287800	-3.05126700
C	-1.79968700	1.34389500	-4.16178300
C	-2.23576700	1.98245400	-5.34149000
C	-2.92940100	1.19842200	-6.24414300
H	-2.04179000	3.05189800	-5.50998100
N	0.45949600	-2.10609800	-1.18772300
C	1.39946400	-3.08369600	-1.29259600
N	1.06214400	-1.02536800	-0.69977500
C	1.30370300	-4.42691900	-1.71244200
C	2.46694300	-5.17048400	-1.66465000
H	0.34294800	-4.84803700	-2.04336600
N	2.35654500	-1.23704900	-0.48498500
C	2.62564300	-2.53645900	-0.84872100
C	3.80327500	-3.30649500	-0.80104000
C	3.72212500	-4.63345000	-1.21524200
H	4.74849700	-2.85810700	-0.46404100
H	-2.93287900	-1.88629200	-4.66102800
H	4.65659500	0.11427700	3.42583700
C	-3.99516900	7.25943100	2.59495200
C	-3.69944800	7.25931900	3.99295600
C	-5.01405600	8.08186500	2.10822500
C	-4.38506600	8.04394200	4.90862800
H	-2.87998700	6.62014000	4.35377900
C	-5.71880100	8.88245900	3.01985100
H	-5.29097800	8.09585400	1.04476300
C	-5.40697100	8.85987200	4.39722000
H	-4.12687200	8.02564400	5.97702100
H	-6.42716100	10.04546600	5.89858500
C	6.94546800	3.78475500	-3.31003300
C	7.39626000	4.00766300	-4.64628400
C	7.87393600	3.73511400	-2.26732400
C	8.73522900	4.17554000	-4.97045600
H	6.64946600	4.02156200	-5.45417400
C	9.23202500	3.90316400	-2.57593200
H	7.55946400	3.59794300	-1.22285100
C	9.65110600	4.12036600	-3.90765900
H	9.05256600	4.33436600	-6.01096900
H	11.71656300	4.40102500	-4.50538200

C	4.81975100	0.25386900	6.15217300
C	5.11204600	1.06038000	7.29363700
C	6.20297400	0.82962700	8.12013100
H	4.45565200	1.91618100	7.51129200
C	5.65358400	-0.82173600	5.83681500
C	7.02717800	-0.25614100	7.78437300
H	6.40677200	1.47588400	8.98576800
C	6.76107800	-1.07070600	6.66103800
H	5.44606100	-1.48338600	4.98398400
C	-6.07200600	-3.91221600	1.84163500
C	-5.72038100	-5.20183700	1.33672600
C	-6.63090700	-6.24360900	1.26516800
H	-4.68265300	-5.36986600	1.01350400
C	-7.37512200	-3.66660100	2.28855700
C	-7.94110700	-5.99782200	1.71104900
H	-6.34952100	-7.23475600	0.88266700
C	-8.29136800	-4.72435400	2.21299800
H	-7.67024800	-2.67242300	2.65333700
H	-10.27297900	-4.19990100	2.92300000
C	-3.96095700	-0.97287700	-7.04532900
C	-3.75163400	-0.72526400	-8.43658000
C	-4.42043300	-1.43029100	-9.42472900
H	-3.01186200	0.03504000	-8.72700700
C	-4.86935700	-1.95638800	-6.63794500
C	-5.33319300	-2.41811700	-9.01723500
H	-4.24595300	-1.24034900	-10.49309500
C	-5.54051100	-2.66668400	-7.64169100
H	-5.05782300	-2.14369400	-5.57123400
H	-6.91278700	-4.15671400	-6.86750200
C	4.93086500	-5.50127300	-1.19349100
C	5.86500800	-5.38964500	-0.11822100
C	7.01386400	-6.16141700	-0.05040300
H	5.64225800	-4.68221100	0.69402400
C	5.15773600	-6.41793400	-2.22599800
C	7.24542000	-7.07987400	-1.08907000
H	7.72197800	-6.07628800	0.78585000
C	6.32149100	-7.19538400	-2.15187300
H	4.46228900	-6.49774800	-3.07370400
H	6.55283900	-8.56050200	-3.82165100
N	8.28358900	-7.96985100	-1.30184300
N	8.06012000	-8.60864000	-2.40719400
N	6.88540400	-8.16173700	-2.94301100
N	-6.47755100	-3.66646600	-7.64993000
N	-6.81536600	-4.00961800	-8.92775100
N	-6.13990500	-3.27008000	-9.75101000
N	11.39878700	4.10361700	-2.48432600
N	10.34726900	3.90632200	-1.75356500
N	11.01010500	4.23706500	-3.78716700
N	-6.76359600	9.76984600	2.81577200
N	-7.09928100	10.28230400	3.95702500
N	-6.29816900	9.75234800	4.92952100

N	-9.05429700	-6.81840500	1.76042200
N	-10.04573400	-6.14085100	2.24844900
N	-9.61641100	-4.87464000	2.52897600
N	7.73246200	-2.05628900	6.58730100
N	8.55910000	-1.89562100	7.57140400
N	8.15903900	-0.81849500	8.31095400
H	8.70066800	-0.54725200	9.13246800
H	-5.75885300	-2.04636300	3.78644900
H	4.88630700	5.16443600	-4.42567800
H	2.43399400	-6.23162100	-1.95278200
H	2.35891100	1.03180800	7.00238200
H	-3.31350300	1.66298500	-7.16418600
H	-3.22487900	7.84287800	0.06110200
H	4.43756300	-0.95713500	0.70868400
C	5.31980800	1.08726400	0.59695100
C	5.50244900	-0.17885800	-0.07888700
H	5.53029300	-0.23965000	-1.18290800
H	6.20802200	-0.89350200	0.38902900
H	5.15917700	1.98639000	-0.00971100
C	6.08864700	1.43196700	1.85058200
H	6.14778700	0.57404600	2.55271200
H	7.14522200	1.57729100	1.51926400
C	5.62545600	2.71384800	2.54314400
H	6.23608100	2.93049300	3.44158200
H	5.71708400	3.58014300	1.85564900
H	4.56667000	2.65246700	2.85915300

Pcw

Ni-MFU-4l

Zn	21.26265100	9.79941300	5.92350700
Cl	20.06113700	11.08521900	4.61111400
Zn	23.21894700	7.66117200	8.06648200
N	22.52058500	10.62622900	7.28751500
C	22.85381900	11.90102200	7.61960000
N	23.22598900	9.81885500	8.07628600
C	22.40366500	13.12226000	7.07737000
C	22.94287800	14.27123900	7.62280700
H	21.67161600	13.17040700	6.25908000
Zn	21.03292500	5.57779900	10.01319500
Cl	19.70540000	4.28472000	11.18919700
N	20.24544200	6.91181900	8.69342100
C	18.95637100	7.22546900	8.38026100
N	21.04500100	7.67823700	7.95618500
C	17.72811300	6.71728800	8.84979800
C	16.58772800	7.26664000	8.29699700
H	17.66781400	5.92669900	9.61077100
Ni	25.20828000	9.67763700	10.30059600
N	23.88724000	8.37330100	11.02129400
C	23.63111100	8.03833900	12.32633300
N	23.09212300	7.63738500	10.23845700

C	24.16440200	8.47599200	13.55574300
C	23.63164700	7.90627900	14.69382200
N	20.33772600	8.48533700	7.17067000
C	19.01672200	8.24103800	7.39762900
C	17.85133600	8.80037600	6.83529200
C	16.65118000	8.29983100	7.29796700
H	17.88463200	9.58818200	6.06967500
N	23.99312300	10.51626000	8.92403400
C	23.79919000	11.85156100	8.66971400
C	24.33781100	13.02695500	9.22904700
C	23.90449300	14.22035000	8.68928300
H	25.15353100	13.06988700	9.94546200
N	22.31101700	6.83943200	10.96318500
C	22.61200800	7.05899300	12.27054000
C	22.06942200	6.47884900	13.43552600
C	22.59041200	6.91662500	14.63694700
H	21.27660600	5.71839200	13.40136300
N	22.38613900	4.72237300	8.75126300
C	22.66029100	3.41765700	8.46707800
N	23.20359400	5.48071000	8.02622000
C	22.09628500	2.21746600	8.94586200
C	22.62174800	1.04783200	8.43285600
H	21.28320700	2.20140000	9.68518900
Zn	25.37595800	5.60921600	6.05272400
Cl	26.69494700	4.35084200	4.82546500
N	24.12770600	6.93362300	5.14586300
C	23.92462600	7.24378400	3.83402300
N	23.32036200	7.69616000	5.87817800
C	24.50789600	6.74361500	2.65204000
C	24.05828700	7.29621900	1.46990900
N	24.00627600	4.73091900	7.27521800
C	23.70625500	3.42283000	7.51470400
C	24.24096000	2.22720600	6.99294100
C	23.68565700	1.05498700	7.46445000
H	25.05315300	2.21699300	6.25272100
N	22.59350500	8.49714800	5.10388600
C	22.93495900	8.25376600	3.80676500
C	22.47909600	8.81547700	2.59681600
C	23.05234300	8.32396100	1.44025500
H	21.71025800	9.60011900	2.56309700
N	26.19075200	6.86247400	7.42766800
C	27.47480000	7.09682600	7.81542200
N	25.39624000	7.62197500	8.18246800
C	28.69606500	6.55974600	7.35870500
C	29.83970100	7.02435300	7.97882700
H	28.74830500	5.81601700	6.55109100
N	26.09852500	8.34706200	9.04364100
C	27.42193100	8.05169900	8.85733500
C	28.58978200	8.50203500	9.50286200
C	29.78335000	7.98754100	9.04357300
H	28.59846700	9.22818800	10.32365000

H	25.27725400	5.95892000	2.65934000
C	23.18982400	8.38012400	-0.91911900
C	24.18591300	7.36190900	-0.88856500
C	22.75279800	8.92778200	-2.11100200
C	24.76688000	6.86877800	-2.04723500
C	23.33152700	8.43901600	-3.29629200
C	24.31874000	7.42878900	-3.25342600
H	25.53109700	6.08357600	-1.97703600
C	32.19635000	6.98264700	8.15311000
C	32.14063000	7.94564000	9.20207200
C	33.40123400	6.47326300	7.70489200
C	33.28544400	8.41989000	9.82473600
C	34.57257100	6.94353100	8.32548200
C	34.50442500	7.89886000	9.36451800
H	33.19650900	9.15985000	10.63101000
C	14.29070400	8.34688100	7.20574400
C	14.22659200	7.32373900	8.19501700
C	13.14851100	8.89949000	6.64621100
C	13.01665400	6.83048100	8.64694800
C	11.92383400	8.39446200	7.10925500
C	11.84757700	7.37999700	8.09012700
H	12.98579600	6.04170800	9.40977800
C	22.60354200	-1.31566700	8.38420700
C	23.65745300	-1.30739900	7.42557900
C	22.05888900	-2.49848600	8.84886600
C	24.19035000	-2.47956300	6.91057000
C	22.58752000	-3.69726100	8.33677600
C	23.63313500	-3.67639600	7.38636200
H	25.00225500	-2.42630400	6.17336600
O	31.04330900	6.52965100	7.55274100
O	30.93540500	8.43361100	9.64449300
H	33.42610700	5.73163600	6.89594100
N	35.89879200	6.62663400	8.09905900
N	35.81985500	8.08939700	9.69222100
N	36.63482700	7.31287100	8.91678600
O	22.09512300	-0.13452700	8.87738200
O	24.18709100	-0.12435500	6.97387300
H	21.24697700	-2.48629900	9.58757400
N	22.25604700	-5.01225200	8.60433500
N	23.85722600	-5.00567800	7.14822100
N	23.01652300	-5.78493100	7.89273700
C	23.63027400	7.76263300	17.05262700
C	22.59540500	6.78449900	16.99687100
C	24.16524500	8.19610900	18.25668200
C	22.07305300	6.21933600	18.14561600
C	23.63059400	7.61845700	19.41846800
C	22.60413800	6.64822300	19.37553700
H	21.27575600	5.46733300	18.08364000
O	22.08380100	6.37312100	15.78725300
O	24.13837300	8.31631900	15.90315500
H	24.96131000	8.95228300	18.25436600

N	23.86404000	7.75833100	20.76015500
N	22.29189200	6.27373500	20.66894800
N	23.04621400	6.93905400	21.48732400
H	24.95823200	9.22705200	13.63857500
O	22.63075600	8.84933200	0.24881600
O	24.60882400	6.82827900	0.30315900
H	21.98432500	9.71164600	-2.11589600
N	24.61804400	7.23671700	-4.57534600
N	23.87445100	8.06289900	-5.37075100
N	23.10459100	8.78328000	-4.61561200
O	15.37926900	6.79418800	8.73182300
H	13.24482700	9.68605100	5.88625200
O	15.50010000	8.82560500	6.76759400
N	10.60828600	8.65194800	6.83193300
N	10.51683800	7.09773400	8.33530400
N	9.78554300	7.85924100	7.58218600
C	23.05992300	16.63156900	7.64155300
C	24.01869400	16.58063800	8.69439900
C	22.62967100	17.83573800	7.11540500
C	24.56803400	17.72939700	9.24367700
C	23.17665600	19.01113700	7.66079600
C	24.12697900	18.94775700	8.70476400
H	25.30567400	17.64348800	10.05242900
O	22.53411200	15.47487300	7.11194800
O	24.44650600	15.37643000	9.19824500
H	21.89098500	17.85675200	6.30368700
N	22.94733900	20.33803400	7.34842300
N	23.68143600	21.07888000	8.11895200
N	24.40377400	20.26630700	8.94763700
H	24.52931700	8.36069900	21.24579500
H	10.20029100	9.31932200	6.17649800
H	24.53094600	-5.45014700	6.52375700
H	36.23323100	8.69958400	10.39805900
H	25.04051300	20.68321200	9.62737600
H	25.28432300	6.59395800	-5.00472000
C	25.70217700	11.07518500	11.61891700
H	26.17450300	11.75177500	10.85948500
C	26.85371000	10.51790300	12.48811000
H	27.16118200	9.48924900	12.17522600
C	28.10221800	11.41009800	12.49134300
H	28.90178600	11.00979000	13.14895800
H	28.52520300	11.50623800	11.46854200
H	26.50357800	10.39298700	13.53691000
H	27.85494700	12.43440300	12.83899300
C	24.65011800	11.84617400	12.40272300
H	23.88483000	12.30033500	11.74223100
H	24.10287000	11.18664000	13.10798900
H	25.08542700	12.67295800	13.01442100

Ni-CFA-1

Zn	-0.12868100	3.39401100	-2.56220000
Cl	-0.29722800	5.04759100	-3.97537700
Zn	0.18626300	0.69536400	-0.25040800
N	1.70291700	2.72969300	-2.01462100
C	2.93998100	3.18163200	-2.35178900
N	1.85987100	1.71186000	-1.18109200
C	3.35963100	4.23639400	-3.18947900
C	4.72239200	4.43547600	-3.29549900
H	2.62801900	4.86003500	-3.70720800
Zn	-1.41276000	1.61178700	2.82977500
Cl	-2.36524100	2.18830600	4.70833800
N	-1.41715400	2.93189200	1.29688300
C	-1.93660800	4.18713100	1.18021700
N	-0.82983100	2.62658700	0.15289900
C	-2.66277900	4.98374400	2.08456700
C	-3.05983000	6.24513000	1.64688100
H	-2.91314800	4.59438500	3.07284300
Ni	3.67167400	-0.04084500	0.30341500
N	2.42809100	0.51255400	1.86544200
C	2.68302700	0.65035000	3.20376000
N	1.14879400	0.80323700	1.68806800
C	3.86313100	0.47209900	3.94968800
C	3.80173800	0.69809800	5.32221300
N	-0.93227200	3.61376700	-0.71824300
C	-1.62248000	4.62771900	-0.12508500
C	-2.01740700	5.90369800	-0.57829100
C	-2.72331000	6.68241700	0.31886300
H	-1.76026400	6.24454900	-1.58311100
N	3.13868400	1.45027100	-0.94689000
C	3.86557400	2.36558900	-1.66219400
C	5.25008900	2.58658200	-1.77984800
C	5.68139400	3.62666400	-2.59778500
H	5.95622700	1.94738500	-1.25895900
N	0.54845800	1.12976500	2.82232600
C	1.47400500	1.05110900	3.81675900
C	1.39788000	1.28641600	5.20534600
C	2.56303400	1.10416200	5.92610400
H	0.45607400	1.58602700	5.66952400
N	-2.11708000	0.00366500	1.81888300
C	-3.14944100	-0.85303900	2.05654100
N	-1.54503100	-0.35450500	0.68295000
C	-4.08829600	-0.94328300	3.10505900
C	-5.01637300	-1.96296700	3.01128500
H	-4.06067900	-0.24327200	3.94249300
Zn	-1.45837700	-2.17673500	-1.58482300
Cl	-2.48339300	-3.93228100	-2.39019000
N	-1.43967000	-0.48331600	-2.68484200
C	-1.95955900	-0.17644800	-3.90681100
N	-0.85864500	0.60152600	-2.20553500
C	-2.66478300	-0.95518800	-4.84215000
C	-3.06584200	-0.32870100	-6.01981100

N	-2.14391400	-1.40564200	0.15388800
C	-3.16724900	-1.76708000	0.97908000
C	-4.11851700	-2.79991900	0.88926000
C	-5.05403200	-2.89493700	1.91706100
H	-4.11742000	-3.46933100	0.02741600
N	-0.96319100	1.61493200	-3.04611600
C	-1.65065900	1.18265300	-4.14032100
C	-2.05038200	1.82662000	-5.32980700
C	-2.74991100	1.05669200	-6.23995100
H	-1.81890900	2.87986800	-5.50032300
N	0.50895900	-2.26082600	-1.12724000
C	1.38968900	-3.29154100	-1.21735600
N	1.16636300	-1.20834700	-0.66300800
C	1.22433600	-4.62681000	-1.64057800
C	2.34580900	-5.43048000	-1.59692000
H	0.24838300	-4.98896500	-1.97024900
N	2.44745200	-1.47584200	-0.44701400
C	2.63704100	-2.79533600	-0.77252600
C	3.76946700	-3.63376800	-0.73057700
C	3.62319700	-4.95410600	-1.14761500
H	4.73375100	-3.25208700	-0.40721300
H	-2.85561500	-2.01062500	-4.64073800
H	4.79610500	0.19219500	3.45872300
C	-3.83456700	7.14260100	2.54625000
C	-3.55696200	7.15401500	3.94791300
C	-4.84096900	7.96759700	2.03833900
C	-4.24860400	7.95246200	4.84695300
H	-2.75234800	6.52004900	4.32589600
C	-5.55168800	8.78197400	2.93296300
H	-5.10332500	7.97375200	0.97957300
C	-5.25788000	8.77060900	4.31443100
H	-4.00723000	7.94339800	5.91139100
H	-6.28913000	9.97537900	5.77797400
C	7.13707800	3.90091500	-2.73952300
C	7.67673400	4.26705800	-4.00978500
C	7.98801700	3.78727300	-1.63725500
C	9.02706400	4.51684600	-4.21145400
H	7.00141800	4.32813700	-4.86588100
C	9.35605000	4.03618400	-1.82151600
H	7.61219700	3.53330000	-0.64514500
C	9.86310300	4.39602900	-3.09010400
H	9.41116800	4.78423300	-5.19757100
H	11.94485000	4.80677200	-3.48545200
C	5.01452100	0.51212100	6.16383100
C	5.30138500	1.43062200	7.21877500
C	6.42364000	1.32113500	8.02798400
H	4.62156300	2.27018400	7.37929500
C	5.88551500	-0.55255600	5.92100800
C	7.28516400	0.24397500	7.76584100
H	6.62241000	2.04576300	8.81970400
C	7.02450400	-0.68027400	6.72958200

H	5.68733700	-1.28990100	5.14178800
C	-6.09620000	-3.95649300	1.88399700
C	-5.76893300	-5.25549800	1.38688500
C	-6.69985800	-6.27928600	1.31807000
H	-4.74220300	-5.44915500	1.07096500
C	-7.39542800	-3.68252100	2.32570500
C	-8.00613400	-6.00503700	1.75877200
H	-6.43763900	-7.27022000	0.94378800
C	-8.33239200	-4.72217400	2.25294200
H	-7.67409800	-2.68960800	2.68202600
H	-10.29843100	-4.16487600	2.94987900
C	-3.82549700	-1.08996400	-7.04815700
C	-3.58053000	-0.85957300	-8.43652100
C	-4.25067900	-1.55143400	-9.43302700
H	-2.81760600	-0.13170400	-8.71906500
C	-4.77193400	-2.04171700	-6.65230300
C	-5.20162100	-2.50747600	-9.03716400
H	-4.04939300	-1.37526400	-10.49100700
C	-5.44446300	-2.73878700	-7.66441800
H	-4.99035000	-2.21533600	-5.59755200
H	-6.87276400	-4.17506100	-6.91909000
C	4.79419200	-5.87238400	-1.13551900
C	5.74059200	-5.80404500	-0.06740300
C	6.85822000	-6.62122100	-0.01216200
H	5.55883500	-5.09732900	0.74447500
C	4.97603500	-6.79234300	-2.17387700
C	7.04426400	-7.54317800	-1.05664200
H	7.57079900	-6.56635300	0.81250200
C	6.10815600	-7.61620400	-2.11257000
H	4.28004600	-6.84200400	-3.01275100
H	6.27812100	-8.97691600	-3.77999200
N	8.03675700	-8.47103700	-1.28667500
N	7.77868200	-9.08730100	-2.38390200
N	6.62661700	-8.59726700	-2.90801400
N	-6.40798800	-3.70570500	-7.68720900
N	-6.72539300	-4.04273200	-8.96223000
N	-6.01848200	-3.33880900	-9.77223800
N	11.48673100	4.30938500	-1.54740900
N	10.40510700	4.00521500	-0.92581100
N	11.19749100	4.55127100	-2.85126200
N	-6.58289900	9.67218200	2.71423600
N	-6.92457400	10.19141600	3.83785500
N	-6.14746100	9.67168300	4.82211700
N	-9.13435100	-6.79439300	1.81163600
N	-10.10263700	-6.09812000	2.28940000
N	-9.65603500	-4.84647700	2.56427900
N	8.03335100	-1.62123200	6.72085200
N	8.86938800	-1.33720100	7.65294300
N	8.44995700	-0.22157500	8.30221600
H	9.00080900	0.14048600	9.07139000
H	-5.74197600	-2.08561200	3.81775300

H	5.08746400	5.25921000	-3.91229900
H	2.25583000	-6.47869800	-1.88860600
H	2.54002200	1.25035400	7.00796700
H	-3.10059700	1.52567800	-7.16121000
H	-3.02267100	7.68759900	0.01597000
C	5.52476300	-0.67231100	0.00128700
C	6.50154300	0.20440400	0.80618300
H	6.91752300	1.00039900	0.15015300
H	5.97577500	0.75621100	1.62232700
C	7.66612800	-0.57772100	1.43494900
H	8.37577900	0.09261900	1.96181100
H	7.29511500	-1.32004300	2.17282700
H	8.23653100	-1.13406100	0.66338400
H	5.37188000	-1.61911400	0.58729600
C	6.00028300	-1.00533900	-1.40465600
H	5.29104800	-1.66531000	-1.94304400
H	6.10878100	-0.08873300	-2.02143200
H	6.99258800	-1.51530600	-1.41933100

AE2

Ni-MFU-4l

Zn	21.40695600	9.71006900	5.68329700
Cl	20.18441900	11.04494300	4.44023900
Zn	23.39509300	7.53433100	7.74369200
N	22.73107200	10.49538300	7.01649200
C	23.00163200	11.78508300	7.36098600
N	23.50024600	9.70289200	7.76311100
C	22.47369800	13.00523200	6.89132000
C	22.97159700	14.15293600	7.47535900
H	21.70703400	13.05098200	6.10487900
Zn	21.24892700	5.53093400	9.81397200
Cl	19.94175000	4.30493900	11.08085800
N	20.42451200	6.86344700	8.50780300
C	19.13008200	7.18492500	8.22637400
N	21.21076500	7.61483100	7.74042500
C	17.91093600	6.70036000	8.74271700
C	16.76091500	7.25920100	8.22043200
H	17.86567100	5.92211800	9.51749400
Ni	25.53199000	9.55211900	9.86605800
N	24.19128400	8.30542900	10.66413300
C	23.85683800	8.09097700	11.97166000
N	23.41935200	7.52583200	9.91566400
C	24.33761500	8.65220100	13.17241600
C	23.75759900	8.19899500	14.33942900
N	20.48815800	8.41780900	6.96380500
C	19.17210600	8.18724400	7.22931900
C	17.99669400	8.75649800	6.69824200
C	16.80579600	8.27899600	7.20650500
H	18.01669800	9.53731000	5.92491900
N	24.26664100	10.41301300	8.58293600

C	23.98958600	11.73457500	8.37217300
C	24.48905200	12.91037500	8.96880400
C	23.97048100	14.10294000	8.50772000
H	25.24157100	12.88908900	9.76744000
N	22.59111600	6.80274300	10.66961300
C	22.82679400	7.12148900	11.97336500
C	22.23597200	6.65969600	13.16737700
C	22.71560200	7.20876900	14.33989700
H	21.43705500	5.90470000	13.17531800
N	22.51812100	4.61974800	8.50080500
C	22.75272300	3.30505900	8.22771100
N	23.31486500	5.34901600	7.72405900
C	22.19022100	2.12486700	8.75536100
C	22.66982000	0.93609400	8.24128600
H	21.41307300	2.13816100	9.53254200
Zn	25.40228600	5.40384200	5.65588200
Cl	26.65082600	4.11374300	4.39017000
N	24.14776200	6.75831600	4.79040900
C	23.89668700	7.06567400	3.48631300
N	23.39516600	7.54943900	5.55068400
C	24.41414900	6.54118300	2.28444300
C	23.92783700	7.09664300	1.11822100
N	24.06640400	4.57008200	6.94980100
C	23.75219700	3.27292300	7.22739300
C	24.24026600	2.05794700	6.70478500
C	23.68675300	0.90519500	7.22433500
H	25.01705200	2.01894700	5.92826000
N	22.65823100	8.36566900	4.80167500
C	22.93475700	8.10227700	3.49334000
C	22.44077200	8.66655500	2.29967800
C	22.94912300	8.15077000	1.12353800
H	21.69321600	9.47224300	2.29275500
N	26.29922900	6.67597200	6.97705400
C	27.60831100	6.91293200	7.26726000
N	25.56084100	7.46695600	7.75192500
C	28.79222500	6.35400500	6.74485500
C	29.97808200	6.82704500	7.27074500
H	28.78231100	5.58289500	5.96145500
N	26.32001900	8.21808100	8.54315400
C	27.62552600	7.90484100	8.27499800
C	28.84087300	8.38299600	8.80715200
C	29.99999700	7.83465100	8.29497800
H	28.89146200	9.15193900	9.58999900
H	25.16237800	5.73634100	2.26553500
C	22.98119300	8.18233200	-1.24004100
C	23.95060200	7.13828100	-1.24413300
C	22.50413500	8.72985700	-2.41654800
C	24.46441900	6.61859100	-2.42273300
C	23.01463700	8.21438600	-3.62170700
C	23.97598700	7.17866600	-3.61315100
H	25.21035700	5.81396700	-2.37863100

C	32.34032500	6.75983800	7.29669500
C	32.36131700	7.75869600	8.31232500
C	33.50839900	6.21726500	6.79372400
C	33.54790900	8.23698100	8.84739900
C	34.72143700	6.69103200	7.32509200
C	34.72959300	7.68210000	8.33243400
H	33.51718800	9.00756300	9.62909400
C	14.44451100	8.36293100	7.19547000
C	14.39878000	7.35308500	8.19936400
C	13.29234300	8.92871800	6.67058100
C	13.19775800	6.88657100	8.70077900
C	12.07681600	8.45075400	7.18373000
C	12.01880100	7.44960100	8.17939300
H	13.18142100	6.10781400	9.47444300
C	22.60534900	-1.42706400	8.23812200
C	23.61270400	-1.45651600	7.23106300
C	22.06082600	-2.59055600	8.74941900
C	24.09796600	-2.64786000	6.71298100
C	22.54162500	-3.80836400	8.23509700
C	23.54112600	-3.82490100	7.23623900
H	24.87507000	-2.62322600	5.93755000
O	31.14579500	6.30385500	6.78392900
O	31.19210700	8.28885200	8.80224700
H	33.47374300	5.44821600	6.01101700
N	36.02654000	6.34646500	7.02881700
N	36.06500800	7.86362800	8.57201600
N	36.81988300	7.04905000	7.77561600
O	22.14310100	-0.22730900	8.73354300
O	24.14372500	-0.29202200	6.73319800
H	21.28516400	-2.54903700	9.52525600
N	22.19752200	-5.11106600	8.54237600
N	23.72773800	-5.16235500	7.01250300
N	22.90865300	-5.91074300	7.81043400
C	23.64767900	8.30641600	16.69762000
C	22.61705500	7.32226800	16.69865500
C	24.12479000	8.86968700	17.87189600
C	22.04193000	6.88001500	17.87574900
C	23.53676600	8.41636300	19.06269400
C	22.51466400	7.44067900	19.07609300
H	21.24887100	6.12104800	17.85745000
O	22.16229500	6.78048600	15.51672200
O	24.21043100	8.73486800	15.52074300
H	24.92000200	9.62547000	17.82468200
N	23.70652200	8.69966400	20.39113800
N	22.14219000	7.20386100	20.38572100
N	22.85627500	7.95750700	21.16216200
H	25.12286100	9.41878500	13.18883500
O	22.48887500	8.67842500	-0.05258400
O	24.41453700	6.60472600	-0.06702100
H	21.75705300	9.53400700	-2.39448400
N	24.20845600	6.96629900	-4.94527300

N	23.45076400	7.80461400	-5.71381500
N	22.73562100	8.55224600	-4.93235900
O	15.56121900	6.80954700	8.70156400
H	13.37483000	9.70455700	5.89788400
O	15.64556100	8.81558900	6.70755300
N	10.75662400	8.72759800	6.95118800
N	10.69370700	7.19330700	8.47653000
N	9.94901400	7.95758200	7.74006700
C	22.95122600	16.51215900	7.61767000
C	23.93899000	16.46200600	8.64371100
C	22.43625000	17.71448400	7.16921200
C	24.43217000	17.61138300	9.24338300
C	22.92605500	18.89006500	7.76650800
C	23.90514400	18.82796200	8.78350200
H	25.19275700	17.52637400	10.03083600
O	22.47900900	15.35420400	7.04029400
O	24.44229800	15.26066800	9.07783400
H	21.67569800	17.73403200	6.37771300
N	22.60903800	20.21491400	7.53375000
N	23.31728700	20.95586500	8.32764800
N	24.10842200	20.14580000	9.09311300
H	24.34789800	9.35421800	20.84039800
H	10.33596300	9.39430600	6.30284500
H	24.36247200	-5.63161800	6.36545800
H	36.52918000	8.49155200	9.22932400
H	24.73679100	20.56361100	9.78031500
H	24.83725500	6.30214100	-5.39836700
H	25.61132000	10.63117300	10.96134200

Ni-CFA-1

Zn	-0.59760300	2.97388900	-2.72536300
Cl	-0.89653800	4.56629100	-4.20624600
Zn	-0.08427800	0.34616100	-0.32720300
N	1.28151600	2.43108000	-2.17505500
C	2.49645500	2.87993600	-2.60195300
N	1.49419100	1.47196700	-1.27747800
C	2.85188300	3.86535800	-3.54680000
C	4.20342000	4.06145200	-3.75323200
H	2.07890000	4.44400000	-4.07384700
Zn	-1.70897800	1.22704800	2.75525800
Cl	-2.69655500	1.77296300	4.64154500
N	-1.82085300	2.49510100	1.17525400
C	-2.41947900	3.71515900	1.03257800
N	-1.22269700	2.19338800	0.02795700
C	-3.18462800	4.48691600	1.92618600
C	-3.66459900	5.70980900	1.46306000
H	-3.40378800	4.10882800	2.93552400
Ni	3.42910000	-0.10459500	0.24543600
N	2.20945200	0.35053400	1.78276800
C	2.44521500	0.48973600	3.13082200
N	0.91782900	0.57547800	1.57758300

C	3.60530100	0.33125300	3.91423800
C	3.49246000	0.52403100	5.28822500
N	-1.39880500	3.15889400	-0.86746400
C	-2.14703300	4.14213700	-0.28669000
C	-2.62641500	5.37909200	-0.76568400
C	-3.37045700	6.13409700	0.12088500
H	-2.40170000	5.71551400	-1.78836600
N	2.79094900	1.26771400	-1.08257200
C	3.47391000	2.13614900	-1.90139300
C	4.84769000	2.33432200	-2.13961000
C	5.21348600	3.30929900	-3.06293600
H	5.59527700	1.72983400	-1.60746600
N	0.28847200	0.86897000	2.71299900
C	1.20481100	0.82434100	3.72181700
C	1.07735100	1.02927900	5.11156500
C	2.22518400	0.87651100	5.86431900
H	0.10329200	1.28202400	5.55584800
N	-2.29342500	-0.45882300	1.77524900
C	-3.25952700	-1.38546200	2.04098400
N	-1.69737600	-0.80124900	0.63858100
C	-4.18412400	-1.51547700	3.09796000
C	-5.03695300	-2.60112900	3.03656000
H	-4.20429100	-0.78966300	3.92404700
Zn	-1.52261700	-2.71025100	-1.59041000
Cl	-2.42923100	-4.56201000	-2.35558500
N	-1.60858300	-1.02190900	-2.71475700
C	-2.16177800	-0.78116200	-3.94022400
N	-1.10246200	0.11972300	-2.26124000
C	-2.81708000	-1.63271400	-4.84803200
C	-3.27538700	-1.06699900	-6.03552200
N	-2.22576300	-1.91425900	0.14141200
C	-3.21618500	-2.32637600	0.98755000
C	-4.09160200	-3.42651500	0.93054500
C	-5.01300900	-3.56134700	1.96661900
H	-4.05129300	-4.12411100	0.08112900
N	-1.29326000	1.10384900	-3.13286400
C	-1.95672000	0.59078100	-4.21000700
C	-2.41494600	1.17377200	-5.40989200
C	-3.06492200	0.33199300	-6.29273600
H	-2.26375300	2.24428700	-5.61185600
N	0.45704500	-2.63890400	-1.14897000
C	1.44265200	-3.57582200	-1.25229600
N	1.00498700	-1.51739100	-0.68787900
C	1.42664300	-4.91928300	-1.68059600
C	2.63604900	-5.58701400	-1.65724600
H	0.49020200	-5.39808400	-2.00264200
N	2.30796200	-1.66313000	-0.47866200
C	2.63677200	-2.95496600	-0.82037100
C	3.86296700	-3.64644700	-0.80313800
C	3.86219100	-4.97332200	-1.22745800
H	4.78982000	-3.14359800	-0.49116100

H	-2.93067400	-2.70303500	-4.62172200
H	4.56846700	0.09916700	3.43853700
C	-4.48404300	6.57963600	2.34985900
C	-4.19026500	6.64600100	3.74666800
C	-5.54718700	7.32527400	1.83494100
C	-4.92018500	7.42274800	4.63440300
H	-3.33599100	6.06783900	4.12903200
C	-6.29728900	8.11647700	2.71814500
H	-5.82314500	7.28594800	0.77185600
C	-5.98613600	8.16065500	4.09515500
H	-4.66232800	7.45746200	5.70245400
H	-7.07326700	9.33960800	5.55420100
C	6.65308900	3.58308000	-3.32048400
C	7.10653900	3.85234900	-4.64730100
C	7.57030200	3.57291200	-2.26641000
C	8.43656900	4.10651000	-4.95179400
H	6.37111200	3.83356100	-5.46553300
C	8.91916100	3.82858600	-2.55521000
H	7.25516100	3.39612700	-1.22839200
C	9.34074200	4.09172200	-3.87788000
H	8.75606900	4.29990700	-5.98575300
H	11.39195100	4.50835100	-4.44430800
C	4.68377300	0.35535500	6.16385700
C	4.91271300	1.26272900	7.24228300
C	6.01092300	1.16853300	8.08571900
H	4.19907200	2.08656400	7.39295500
C	5.58985000	-0.68188000	5.93216200
C	6.90819300	0.11835400	7.83443500
H	6.16560000	1.89062100	8.90008200
C	6.70524700	-0.79438000	6.77538300
H	5.43430000	-1.41406900	5.12738400
C	-5.97697700	-4.69487000	1.96735700
C	-5.56030700	-5.97979100	1.50155100
C	-6.41632200	-7.06855400	1.46480800
H	-4.51564900	-6.10465900	1.18110400
C	-7.29038900	-4.50249000	2.41019700
C	-7.73682000	-6.87639800	1.90653700
H	-6.08494400	-8.05544200	1.11257300
C	-8.15133700	-5.60757300	2.36986900
H	-7.63558600	-3.51397800	2.74522400
H	-10.15636300	-5.16368900	3.06918600
C	-3.98679700	-1.90785900	-7.03599700
C	-3.77442000	-1.69405500	-8.43236100
C	-4.40085900	-2.45867000	-9.40381700
H	-3.06640200	-0.91063200	-8.74001400
C	-4.85479200	-2.91784000	-6.60600700
C	-5.27284600	-3.47336500	-8.97366100
H	-4.22399700	-2.29424100	-10.47599700
C	-5.48341900	-3.68816300	-7.59292000
H	-5.04581400	-3.08007900	-5.53563900
H	-6.79681900	-5.21308100	-6.78493800

C	5.12584200	-5.75879600	-1.24330800
C	6.06864600	-5.60898800	-0.18080900
C	7.26761000	-6.30327800	-0.14950500
H	5.81422600	-4.93566200	0.65094300
C	5.39410500	-6.63503900	-2.30068700
C	7.54095600	-7.18016600	-1.21321700
H	7.98335600	-6.18906200	0.67663000
C	6.60825000	-7.33394300	-2.26370100
H	4.69047900	-6.74221300	-3.13859700
H	6.90138400	-8.64256200	-3.96877900
N	8.63222300	-7.99359200	-1.46344000
N	8.43245100	-8.62091700	-2.57962000
N	7.22144500	-8.24226300	-3.08616000
N	-6.37510500	-4.72849300	-7.57824000
N	-6.68378100	-5.12577500	-8.84766400
N	-6.03313500	-4.38286800	-9.68756900
N	11.06794600	4.16164100	-2.43139000
N	10.02217300	3.88863900	-1.71806400
N	10.68810900	4.29041900	-3.73808200
N	-7.39049500	8.93533200	2.48358200
N	-7.75585700	9.46823200	3.60615700
N	-6.92704700	9.01961600	4.59613900
N	-8.80639000	-7.75094500	1.98432500
N	-9.83057700	-7.11020800	2.45393600
N	-9.46652600	-5.81563300	2.69402300
N	7.74010200	-1.71607900	6.77924400
N	8.54695100	-1.42687500	7.75020100
N	8.07095800	-0.32579300	8.40484800
H	8.58821700	0.04341300	9.20348500
H	-5.75533800	-2.75835800	3.85464000
H	4.52764400	4.83969800	-4.45993900
H	2.66656200	-6.64521100	-1.95607500
H	2.16813500	0.99943500	6.95608900
H	-3.46214600	0.75030300	-7.22921700
H	-3.74133200	7.11809600	-0.20171400
H	4.72603700	0.56415500	0.72494200

RI

Ni-MFU-4l

Zn	21.40940800	9.70694300	5.68517100
Cl	20.17437100	11.02331400	4.43290200
Zn	23.39182700	7.55237200	7.74317500
N	22.71692500	10.50026500	7.01651800
C	23.00168900	11.78509700	7.36090500
N	23.47214300	9.70493200	7.77537300
C	22.47367000	13.00523100	6.89134100
C	22.97158800	14.15293500	7.47537100
H	21.70607700	13.05281300	6.10612400
Zn	21.25667800	5.53889400	9.80714700
Cl	19.95534700	4.31708900	11.08711400
N	20.42473500	6.85621900	8.49951900

C	19.13006600	7.18490800	8.22636100
N	21.21034700	7.60394300	7.72844400
C	17.91093500	6.70036500	8.74272000
C	16.76091500	7.25920400	8.22043500
H	17.86498300	5.92142600	9.51653200
Ni	25.68940600	9.63333100	9.76644400
N	24.13996300	8.36865700	10.65680500
C	23.85674400	8.09098600	11.97157700
N	23.37100100	7.58661700	9.91532600
C	24.33766900	8.65219400	13.17240300
C	23.75761400	8.19897400	14.33942900
N	20.48816300	8.41113500	6.95723300
C	19.17210100	8.18725500	7.22933400
C	17.99669300	8.75649200	6.69824000
C	16.80579500	8.27899500	7.20650300
H	18.01670400	9.53594700	5.92367300
N	24.24133600	10.40970600	8.59107900
C	23.98957100	11.73452000	8.37220500
C	24.48900800	12.91037700	8.96881600
C	23.97050500	14.10294500	8.50770800
H	25.26323800	12.89654300	9.74542900
N	22.57199900	6.82466700	10.66789000
C	22.82677300	7.12152400	11.97335200
C	22.23598800	6.65968300	13.16737900
C	22.71560100	7.20876800	14.33989700
H	21.43341400	5.90850100	13.17558900
N	22.53078200	4.62100800	8.51217600
C	22.75270600	3.30505500	8.22770100
N	23.33490000	5.35120400	7.74305400
C	22.19022100	2.12486800	8.75536400
C	22.66982300	0.93609400	8.24128900
H	21.41462300	2.13740900	9.53389500
Zn	25.39794700	5.41384000	5.66090600
Cl	26.63905400	4.10718100	4.40252200
N	24.13864600	6.75224500	4.79121800
C	23.89669300	7.06568300	3.48630600
N	23.38356400	7.54136000	5.55089600
C	24.41414000	6.54117600	2.28444300
C	23.92783400	7.09663900	1.11822100
N	24.07846300	4.57122800	6.96208300
C	23.75220600	3.27291700	7.22740000
C	24.24025900	2.05794700	6.70478200
C	23.68675200	0.90519500	7.22433300
H	25.01823200	2.01911900	5.92958200
N	22.65246600	8.36146400	4.80141900
C	22.93475700	8.10228700	3.49333200
C	22.44076200	8.66654600	2.29967700
C	22.94911900	8.15076600	1.12353800
H	21.69239100	9.47131900	2.29256700
N	26.29924700	6.70347300	6.94645400
C	27.60832700	6.91291500	7.26726600

N	25.56139900	7.53878600	7.68138300
C	28.79222300	6.35401500	6.74483300
C	29.97808200	6.82706300	7.27073100
H	28.78304600	5.58758200	5.95701500
N	26.32727500	8.28637300	8.45944700
C	27.62549900	7.90481900	8.27512100
C	28.84089200	8.38299600	8.80708700
C	30.00000200	7.83468300	8.29495700
H	28.92248400	9.20350400	9.52236300
H	25.16109600	5.73537600	2.26483400
C	22.98119500	8.18233400	-1.24004100
C	23.95060400	7.13828300	-1.24413300
C	22.50413600	8.72985800	-2.41654800
C	24.46442000	6.61859200	-2.42273300
C	23.01463600	8.21438500	-3.62170700
C	23.97598600	7.17866600	-3.61315100
H	25.21027500	5.81404900	-2.37898900
C	32.34032400	6.75983500	7.29669800
C	32.36131800	7.75869200	8.31233300
C	33.50839900	6.21726200	6.79372600
C	33.54791000	8.23697800	8.84740000
C	34.72143700	6.69103300	7.32509100
C	34.72959300	7.68210100	8.33243300
H	33.51796600	9.00947300	9.62704900
C	14.44451100	8.36293000	7.19546900
C	14.39878000	7.35308600	8.19936500
C	13.29234300	8.92871800	6.67058100
C	13.19775800	6.88657100	8.70077900
C	12.07681600	8.45075400	7.18373000
C	12.01880100	7.44960100	8.17939300
H	13.18111200	6.10773900	9.47420100
C	22.60535000	-1.42706400	8.23812300
C	23.61270400	-1.45651600	7.23106300
C	22.06082600	-2.59055600	8.74941900
C	24.09796600	-2.64786000	6.71298100
C	22.54162500	-3.80836400	8.23509700
C	23.54112600	-3.82490100	7.23623900
H	24.87497900	-2.62357500	5.93762900
O	31.14632700	6.30596200	6.78250500
O	31.19244400	8.29544900	8.79543800
H	33.47390400	5.44898200	6.01042500
N	36.02705700	6.34720500	7.02893600
N	36.06501500	7.86432700	8.57214500
N	36.82059300	7.05027600	7.77546900
O	22.14395100	-0.22746100	8.73350700
O	24.14357900	-0.29222900	6.73404100
H	21.28525200	-2.54937600	9.52520700
N	22.19807500	-5.11153900	8.54213300
N	23.72823800	-5.16232100	7.01220500
N	22.90906200	-5.91138400	7.80975500
C	23.64768000	8.30641200	16.69762000

C	22.61704900	7.32227400	16.69865500
C	24.12479200	8.86968600	17.87189600
C	22.04192600	6.88001900	17.87574900
C	23.53676700	8.41636200	19.06269400
C	22.51466400	7.44067900	19.07609300
H	21.24877200	6.12130600	17.85757000
O	22.16219700	6.78176300	15.51699900
O	24.20954900	8.73614000	15.51993100
H	24.91986300	9.62553500	17.82592000
N	23.70688600	8.70018700	20.39104900
N	22.14256100	7.20433500	20.38612600
N	22.85680500	7.95808800	21.16255700
H	25.11043300	9.42902800	13.21960900
O	22.48909400	8.67772900	-0.05292500
O	24.41390900	6.60500300	-0.06728500
H	21.75712600	9.53392300	-2.39470200
N	24.20882400	6.96583100	-4.94523900
N	23.45123400	7.80392600	-5.71451200
N	22.73606000	8.55181400	-4.93285400
O	15.56099200	6.80985100	8.70103000
H	13.37450100	9.70433200	5.89780700
O	15.64520700	8.81494400	6.70783400
N	10.75667600	8.72788200	6.95067400
N	10.69325300	7.19352600	8.47590500
N	9.94839600	7.95874400	7.74007700
C	22.95121900	16.51215800	7.61767700
C	23.93900100	16.46200800	8.64370300
C	22.43624400	17.71448400	7.16921700
C	24.43217400	17.61138400	9.24337800
C	22.92605400	18.89006500	7.76650900
C	23.90514400	18.82796200	8.78350200
H	25.19401900	17.52706100	10.02949500
O	22.48004900	15.35519100	7.04008200
O	24.44471200	15.26159600	9.07534700
H	21.67618300	17.73413000	6.37742500
N	22.60971100	20.21542600	7.53401300
N	23.31819000	20.95668400	8.32787700
N	24.10895800	20.14582500	9.09339000
H	24.34828500	9.35465800	20.84013800
H	10.33661900	9.39438800	6.30197800
H	24.36290400	-5.63101100	6.36491300
H	36.52875400	8.49307300	9.22870900
H	24.73822100	20.56316800	9.77976100
H	24.83775700	6.30162800	-5.39770200
H	26.58579000	10.88143300	9.38324500
C	26.89624200	8.42806300	10.99977100
H	26.18388600	7.92917600	11.66494700
H	27.54373900	7.73907600	10.45496900
C	27.29219300	9.72054300	11.27732500
H	28.19758500	10.18891100	10.86956300
H	26.78284900	10.32329000	12.04990500

Ni-CFA-1

Zn	-0.24727000	3.57299400	-2.61796500
Cl	-0.48522500	5.23831800	-4.02896100
Zn	0.14703700	0.81478100	-0.31852400
N	1.59905700	2.85398700	-2.19832900
C	2.84982400	3.29122300	-2.52867500
N	1.75193000	1.73923900	-1.48304300
C	3.25296900	4.25783700	-3.47354100
C	4.61140100	4.37166400	-3.69845600
H	2.50859500	4.86945500	-4.00487200
Zn	-1.42696400	1.70991600	2.82043700
Cl	-2.37783700	2.26250200	4.72403400
N	-1.43880300	3.04599800	1.29169700
C	-2.00555200	4.28716200	1.18128500
N	-0.83796900	2.76010200	0.13974900
C	-2.72610500	5.06918500	2.10256100
C	-3.13891400	6.33157100	1.68240200
H	-2.96032300	4.67103400	3.10077600
Ni	3.62387500	0.13458300	0.23468500
N	2.38327700	0.48994600	1.83171500
C	2.66978700	0.69781200	3.16211500
N	1.12209400	0.83293300	1.63542100
C	3.81778100	0.40315800	3.92070000
C	3.72817000	0.52263500	5.30457100
N	-0.98436400	3.75593600	-0.72880000
C	-1.71212100	4.74236000	-0.12387500
C	-2.12369500	6.01907100	-0.55948700
C	-2.82366100	6.78385800	0.35433800
H	-1.87907200	6.37777300	-1.57001900
N	3.02658300	1.43129100	-1.33414000
C	3.78812300	2.48433200	-1.84589100
C	5.16787700	2.59939500	-2.10299400
C	5.58250600	3.55558700	-3.02603700
H	5.89457200	1.86770800	-1.74356400
N	0.53179700	1.19187000	2.77872600
C	1.45737600	1.08409700	3.77784700
C	1.35267000	1.21215100	5.17883400
C	2.49159300	0.93323200	5.91006100
H	0.39938700	1.49597000	5.64857900
N	-2.10254700	0.09933200	1.77886900
C	-3.10189800	-0.79549500	2.02615700
N	-1.52676600	-0.23689400	0.62969200
C	-4.03601300	-0.90932700	3.07675100
C	-4.94311300	-1.94739700	2.98094700
H	-4.02403600	-0.20725300	3.92326500
Zn	-1.43011700	-2.10624500	-1.64325200
Cl	-2.45687500	-3.87143200	-2.46073700
N	-1.46291700	-0.36810700	-2.69981200
C	-1.98086300	-0.06932200	-3.92541400
N	-0.92808700	0.74043800	-2.20375600

C	-2.68003000	-0.86222400	-4.85342900
C	-3.11772700	-0.24109500	-6.02081500
N	-2.10087600	-1.31332400	0.10629600
C	-3.10305700	-1.70561800	0.94510700
C	-4.03372300	-2.75707000	0.85310300
C	-4.96456900	-2.87520600	1.88264300
H	-4.02689100	-3.42845900	-0.01815900
N	-1.05996100	1.75622100	-3.04949900
C	-1.71305600	1.29886900	-4.15624800
C	-2.14913600	1.93742800	-5.33595500
C	-2.84277000	1.15339600	-6.23860800
H	-1.95421100	3.00652200	-5.50548100
N	0.54308600	-2.15322800	-1.19173100
C	1.48609500	-3.12872200	-1.28706100
N	1.14489200	-1.06650800	-0.71349000
C	1.39033400	-4.47194400	-1.70690700
C	2.55357400	-5.21550900	-1.65911500
H	0.43023100	-4.89369600	-2.03883300
N	2.43044200	-1.28661900	-0.49464900
C	2.71227400	-2.58148400	-0.84318600
C	3.88990600	-3.35152000	-0.79550500
C	3.80875600	-4.67847600	-1.20970700
H	4.83079000	-2.90128600	-0.45169900
H	-2.84604600	-1.93129600	-4.65515900
H	4.73924900	0.06405900	3.42831500
C	-3.90853800	7.21440600	2.60048700
C	-3.61281700	7.21429300	3.99849100
C	-4.92742500	8.03684000	2.11376000
C	-4.29843500	7.99891700	4.91416300
H	-2.79345000	6.57503300	4.35939700
C	-5.63217000	8.83743300	3.02538600
H	-5.20447500	8.05085800	1.05032300
C	-5.32034000	8.81484700	4.40275500
H	-4.04026500	7.98055600	5.98255600
H	-6.34063200	10.00037200	5.90411800
C	7.03209900	3.73973000	-3.30449800
C	7.48289100	3.96263700	-4.64074900
C	7.96056700	3.69008800	-2.26178900
C	8.82186000	4.13051400	-4.96492100
H	6.73643100	3.97658400	-5.44898200
C	9.31865600	3.85813800	-2.57039700
H	7.64701600	3.55073900	-1.21728200
C	9.73773700	4.07534000	-3.90212400
H	9.13907800	4.28920500	-6.00546100
H	11.80319900	4.35562900	-4.49987400
C	4.90638200	0.20884300	6.15770800
C	5.19867700	1.01535400	7.29917200
C	6.28960500	0.78460100	8.12566600
H	4.54245400	1.87129900	7.51693900
C	5.74021500	-0.86676100	5.84235000
C	7.11380900	-0.30116600	7.78990800

H	6.49352300	1.43099100	8.99118300
C	6.84770900	-1.11573100	6.66657300
H	5.53373900	-1.52694500	4.98802800
C	-5.98537500	-3.95724200	1.84717000
C	-5.63375000	-5.24686300	1.34226100
C	-6.54427600	-6.28863500	1.27070300
H	-4.59602400	-5.41495100	1.01906400
C	-7.28849100	-3.71162600	2.29409200
C	-7.85447600	-6.04284700	1.71658400
H	-6.26283400	-7.27977500	0.88823200
C	-8.20473700	-4.76937900	2.21853300
H	-7.58366400	-2.71748500	2.65895400
H	-10.18631400	-4.24498400	2.92874600
C	-3.87432600	-1.01790200	-7.03979400
C	-3.66500300	-0.77028900	-8.43104500
C	-4.33380200	-1.47531600	-9.41919400
H	-2.92519300	-0.01005500	-8.72159300
C	-4.78272600	-2.00141300	-6.63241000
C	-5.24656200	-2.46314200	-9.01170000
H	-4.15926200	-1.28542800	-10.48755800
C	-5.45388000	-2.71170900	-7.63615600
H	-4.97087200	-2.18908400	-5.56569100
H	-6.82578300	-4.20209800	-6.86194500
C	5.01749600	-5.54629900	-1.18795600
C	5.95163900	-5.43467000	-0.11268600
C	7.10049500	-6.20644300	-0.04486800
H	5.72972500	-4.72524500	0.69811200
C	5.24436700	-6.46296000	-2.22046300
C	7.33205100	-7.12490000	-1.08353500
H	7.80882400	-6.12047300	0.79110300
C	6.40812200	-7.24041000	-2.14633800
H	4.54887500	-6.54295800	-3.06815200
H	6.63935100	-8.60548800	-3.81614800
N	8.37031500	-8.01485000	-1.29653700
N	8.14686300	-8.65373000	-2.40187700
N	6.97206400	-8.20675800	-2.93760100
N	-6.39081400	-3.71157400	-7.64436900
N	-6.72865800	-4.05463300	-8.92217000
N	-6.05322500	-3.31513000	-9.74547300
N	11.48504100	4.05885600	-2.47853600
N	10.43376500	3.86163900	-1.74788400
N	11.09652800	4.19221800	-3.78169200
N	-6.67697400	9.72478100	2.82126700
N	-7.01254400	10.23733000	3.96249300
N	-6.21154900	9.70729500	4.93503800
N	-8.96768600	-6.86341100	1.76591300
N	-9.95908400	-6.18585800	2.25398300
N	-9.52977600	-4.91965300	2.53454400
N	7.81912000	-2.10142400	6.59305800
N	8.64567300	-1.94071300	7.57702200
N	8.24560200	-0.86333100	8.31663000

H	8.78732800	-0.59188000	9.13797900
H	-5.67216400	-2.09137900	3.79203300
H	4.97281900	5.12109900	-4.41836200
H	2.52040300	-6.27655500	-1.94781000
H	2.44560000	0.98728200	7.00791500
H	-3.22652100	1.61787300	-7.15883600
H	-3.13865400	7.79767400	0.06647100
H	4.56305800	-0.89480000	0.92643400
C	4.06341700	2.13023500	0.62979700
H	3.54228100	2.29357900	1.58381000
C	5.24360700	1.51684300	0.70520300
H	6.00575100	1.50790500	-0.08153900
H	5.59906200	1.09196200	1.65476500
H	3.85943700	2.96577300	-0.03168100

TS-RI

Ni-MFU-4l

Zn	21.46590000	9.72198700	5.79738800
Cl	20.25189900	11.07548600	4.56394300
Zn	23.44455800	7.49973300	7.84193900
N	22.72931800	10.49342400	7.18253700
C	23.07256800	11.77618900	7.49296500
N	23.39003000	9.69100300	8.01874400
C	22.52664100	12.99033400	7.03649700
C	23.01084300	14.13590900	7.62817500
H	21.74530200	13.03028000	6.26417300
Zn	21.32665800	5.51606900	9.88870600
Cl	19.99626700	4.30441700	11.14691000
N	20.49397200	6.84564700	8.58553500
C	19.20161200	7.19011700	8.32462800
N	21.27839700	7.58952500	7.81238200
C	17.98644700	6.70300300	8.84091000
C	16.83926300	7.27126000	8.33041500
H	17.94283200	5.91505300	9.60573500
Ni	25.64483100	9.50154800	9.99002400
N	24.26964600	8.27339700	10.75009400
C	23.87035700	8.13767000	12.04441600
N	23.53165600	7.46762800	9.99852100
C	24.27437700	8.74408800	13.25008000
C	23.63918800	8.32344800	14.39703700
N	20.55726200	8.41100600	7.05458000
C	19.24204500	8.20160900	7.34218100
C	18.06896800	8.78018500	6.82300600
C	16.88243300	8.29986500	7.33101100
H	18.08651000	9.56696700	6.05596400
N	24.13161400	10.38589300	8.85808600
C	24.06423800	11.72298600	8.49631500
C	24.54810600	12.90049300	9.09925800
C	24.01117600	14.08688300	8.65209100
H	25.21658600	12.93283900	9.96131500
N	22.66910500	6.77747300	10.74304800

C	22.85038400	7.16161700	12.03430700
C	22.20412600	6.73081300	13.20796500
C	22.61512500	7.32257600	14.38153100
H	21.41396900	5.96671100	13.19922200
N	22.55875100	4.60084300	8.55379700
C	22.79555300	3.28686600	8.27974300
N	23.33345500	5.33085700	7.75795900
C	22.23669700	2.10936500	8.81008300
C	22.70120900	0.92487000	8.28017000
H	21.47127600	2.12093800	9.59856300
Zn	25.41057900	5.38294100	5.68285300
Cl	26.61403300	4.09780300	4.36844300
N	24.18447800	6.77844800	4.84830400
C	23.89664700	7.07739300	3.54695400
N	23.47090400	7.58933800	5.62633100
C	24.38842200	6.55259500	2.33748200
C	23.89435300	7.12328500	1.18537800
N	24.07418400	4.55399900	6.97271800
C	23.77402700	3.25606000	7.26406800
C	24.24650300	2.04503400	6.72534000
C	23.69672800	0.89528400	7.24786500
H	25.00646800	2.00642300	5.93255700
N	22.72331700	8.40868100	4.89010700
C	22.95413500	8.12645800	3.57418400
C	22.45219800	8.70608300	2.39435000
C	22.93538200	8.18966400	1.21132800
H	21.71973400	9.52530000	2.40292500
N	26.33633500	6.58897900	7.02721400
C	27.64698900	6.88197400	7.27559600
N	25.59718500	7.29436200	7.88548700
C	28.82836900	6.34137500	6.73587300
C	30.01136300	6.82371800	7.25260700
H	28.81939000	5.57140700	5.95165600
N	26.35190600	8.01690300	8.69039000
C	27.66454700	7.86172100	8.29093200
C	28.87763000	8.35060500	8.81185900
C	30.03333700	7.82029400	8.28184900
H	28.93894900	9.06987000	9.63626700
H	25.12606200	5.73868300	2.30299900
C	22.93429100	8.23582600	-1.15366000
C	23.88411800	7.17991300	-1.17815200
C	22.44919900	8.79853100	-2.31631300
C	24.37359600	6.65923400	-2.36309300
C	22.93420700	8.28321100	-3.52957100
C	23.87717700	7.23470900	-3.54004100
H	25.10725500	5.84296600	-2.33473600
C	32.37570200	6.78343400	7.25220500
C	32.39677300	7.77170000	8.27233300
C	33.54062900	6.25739000	6.73248800
C	33.57973900	8.25923300	8.79917000
C	34.75185100	6.73998500	7.25438800

C	34.75891600	7.72117400	8.26722300
H	33.54938200	9.02178300	9.58844600
C	14.52001200	8.39130000	7.33219700
C	14.47598100	7.37323100	8.32164400
C	13.37144700	8.96757000	6.81900700
C	13.27935900	6.90485300	8.82400800
C	12.15966400	8.48772200	7.33290200
C	12.10209000	7.47761400	8.31531000
H	13.26426700	6.11727800	9.58851800
C	22.62520600	-1.43928500	8.26392700
C	23.61119400	-1.46741200	7.24182900
C	22.08444900	-2.59974300	8.77841100
C	24.08224200	-2.65378200	6.70760000
C	22.55007100	-3.81441700	8.24873100
C	23.52936200	-3.82846800	7.23410200
H	24.84520900	-2.62818400	5.91856700
O	31.18007300	6.31710700	6.75067800
O	31.22603700	8.28091100	8.78184600
H	33.50587200	5.49355900	5.94487800
N	36.05827100	6.41180400	6.94209100
N	36.09488100	7.91672000	8.49636600
N	36.85138900	7.11722800	7.68665200
O	22.17762800	-0.23990800	8.77341400
O	24.13757700	-0.30183700	6.74150200
H	21.32309200	-2.55915200	9.56814400
N	22.20569500	-5.11830500	8.55440300
N	23.70747400	-5.16558200	6.99740800
N	22.89985200	-5.91641600	7.80440900
C	23.40611800	8.51640900	16.74190300
C	22.39377800	7.51955200	16.72690300
C	23.81545300	9.12979200	17.91298200
C	21.76530500	7.11106600	17.88543300
C	23.17351900	8.71059200	19.08554900
C	22.16776500	7.72216700	19.08425800
H	20.98534200	6.33924700	17.85498300
O	22.00892800	6.92755300	15.54476100
O	24.02440700	8.90770000	15.58086500
H	24.60236500	9.89456800	17.87821800
N	23.27274300	9.04634500	20.40971500
N	21.73195400	7.52756100	20.38218300
N	22.39531700	8.32009900	21.16518600
H	25.06704500	9.50206600	13.28160200
O	22.46797400	8.73174600	0.04447600
O	24.35612500	6.63278300	-0.01035200
H	21.71544300	9.61410600	-2.27858400
N	24.08925300	7.02557800	-4.87678500
N	23.33484700	7.87975300	-5.63063400
N	22.64242300	8.63392200	-4.83490700
O	15.63935500	6.82000400	8.81055600
H	13.45272500	9.75163500	6.05481800
O	15.72083900	8.84441400	6.84371900

N	10.83927100	8.77351800	7.10823700
N	10.77661800	7.22255400	8.61568300
N	10.03149100	7.99885800	7.89211000
C	22.96111700	16.49371900	7.79658000
C	23.95108500	16.44509300	8.81470700
C	22.42836900	17.69080400	7.36390600
C	24.43278300	17.58974600	9.42555000
C	22.90534900	18.86351500	7.97206600
C	23.88788800	18.80168800	8.98164400
H	25.19556400	17.50632800	10.21079900
O	22.49709000	15.33507400	7.21309300
O	24.46170800	15.24267600	9.24247500
H	21.66284900	17.70925200	6.57736100
N	22.56963900	20.18747300	7.75669900
N	23.27179400	20.92778900	8.55661800
N	24.07668900	20.11833700	9.30781500
H	23.88239200	9.72652600	20.86455500
H	10.41962100	9.44930300	6.46896300
H	24.32896000	-5.63202000	6.33588600
H	36.55744400	8.54422700	9.15498200
H	24.70291400	20.53490700	9.99757400
H	24.70137800	6.35387000	-5.34111200
C	26.53850500	10.45423700	8.50460500
H	27.28473800	9.88051400	7.95155800
C	27.04921200	11.10974000	9.66981800
H	28.02167500	10.81638600	10.09142300
H	26.61951500	12.00311800	10.12962000
H	25.89029400	10.99684500	7.81601100
H	26.51691385	10.20955718	11.16202639

Ni-CFA-1

Zn	-0.32601700	3.61660500	-2.62510800
Cl	-0.58848600	5.28440600	-4.03007000
Zn	0.06872000	0.86285500	-0.33139400
N	1.51336300	2.88130600	-2.23166900
C	2.76319300	3.33624800	-2.53421000
N	1.66755400	1.73546400	-1.55832200
C	3.16633800	4.30286200	-3.47907600
C	4.52477000	4.41669000	-3.70399100
H	2.42199200	4.91109800	-4.01427300
Zn	-1.50715400	1.75382600	2.81161800
Cl	-2.45120100	2.30327600	4.72024800
N	-1.51895700	3.09343400	1.28765900
C	-2.09218300	4.33218700	1.17575000
N	-0.91371000	2.80992000	0.13668200
C	-2.81273600	5.11421100	2.09702600
C	-3.22554500	6.37659600	1.67686700
H	-3.04599200	4.71658100	3.09565600
Ni	3.48728900	0.27643200	0.17932700
N	2.30487900	0.50547500	1.83777600
C	2.58315600	0.74283800	3.15658000

N	1.04129100	0.84743300	1.63113400
C	3.73115000	0.44818400	3.91516500
C	3.64153900	0.56766100	5.29903600
N	-1.06401600	3.80431700	-0.73272300
C	-1.79875200	4.78738600	-0.12941000
C	-2.21032600	6.06409600	-0.56502200
C	-2.91029200	6.82888300	0.34880300
H	-1.96480800	6.42259900	-1.57541300
N	2.95200000	1.44399900	-1.40759800
C	3.70149200	2.52935800	-1.85142600
C	5.08124600	2.64442100	-2.10852900
C	5.49587500	3.60061300	-3.03157200
H	5.80506300	1.90039900	-1.76855400
N	0.44866600	1.22440500	2.76910500
C	1.37074500	1.12912300	3.77231200
C	1.26603900	1.25717700	5.17329900
C	2.40496200	0.97825800	5.90452600
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N	-2.18989400	0.14524400	1.77225100
C	-3.18852900	-0.75047000	2.02062200
N	-1.61400400	-0.19037800	0.62315300
C	-4.12264400	-0.86430200	3.07121600
C	-5.02974400	-1.90237200	2.97541200
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Cl	-2.52021100	-3.83718200	-2.46160400
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C	-2.23576700	1.98245400	-5.34149000
C	-2.92940100	1.19842200	-6.24414300
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C	1.39946400	-3.08369600	-1.29259600
N	1.06214400	-1.02536800	-0.69977500
C	1.30370300	-4.42691900	-1.71244200
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C	3.72212500	-4.63345000	-1.21524200

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H	4.65659500	0.11427700	3.42583700
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C	-3.69944800	7.25931900	3.99295600
C	-5.01405600	8.08186500	2.10822500
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H	-2.87998700	6.62014000	4.35377900
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H	-6.42716100	10.04546600	5.89858500
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C	7.87393600	3.73511400	-2.26732400
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H	6.64946600	4.02156200	-5.45417400
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C	4.81975100	0.25386900	6.15217300
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C	6.20297400	0.82962700	8.12013100
H	4.45565200	1.91618100	7.51129200
C	5.65358400	-0.82173600	5.83681500
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H	6.40677200	1.47588400	8.98576800
C	6.76107800	-1.07070600	6.66103800
H	5.44606100	-1.48338600	4.98398400
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C	-5.72038100	-5.20183700	1.33672600
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H	-4.68265300	-5.36986600	1.01350400
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H	-6.34952100	-7.23475600	0.88266700
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C	-3.75163400	-0.72526400	-8.43658000
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C	5.86500800	-5.38964500	-0.11822100
C	7.01386400	-6.16141700	-0.05040300
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C	5.15773600	-6.41793400	-2.22599800
C	7.24542000	-7.07987400	-1.08907000
H	7.72197800	-6.07628800	0.78585000
C	6.32149100	-7.19538400	-2.15187300
H	4.46228900	-6.49774800	-3.07370400
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C	3.90769400	2.18550300	0.59461900
H	3.47818700	2.41040700	1.58528400
C	5.17451500	1.52708600	0.67556000
H	5.92702700	1.55911600	-0.11803200
H	5.61260300	1.34956800	1.67096600
H	3.76911800	3.05462400	-0.04590200

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